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QUANTUM MECHANICS
IN
PHASE SPACE

MASTER OF PHILOSOPHY

PHYSICS

SUBMITTED JUNE 1991

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QUANTUM MECHANICS

IN

PHASE SPACE

ABSTRACT

The objective of this thesis is to describe the fundamental concepts relating to the reformulation of quantum mechanics in phase space. It is assumed that the interested reader is familiar with the principles and techniques of ordinary quantum mechanics.

In classical statistical mechanics the expectation values of physical quantities are calculated as averages over phase space distribution functions. It is possible to obtain a similar procedure in quantum mechanics. However, phase space is a classical concept and thus has no quantum mechanical equivalent, owing to the non-commutability of the operators \hat{p} and \hat{q} . A sensible basic requirement for the formulation of quantum mechanics in phase space is a linear one-one mapping between quantum operators and classical functions. This was achieved by the pioneering work of Weyl, Wigner and Moyal. The phase space that they devised we shall call "pseudo phase space". It is completely quantum. The pseudo phase space variables are represented by commuting c-numbers of momentum, p , and position, q ; they are the result of applying the Weyl correspondence rule to the operators \hat{p} and \hat{q} , respectively.

In some ways the pseudo phase space formulation of quantum mechanics appears to return us to an "almost" classical arena, since we dispense with the calculus of non-commuting operators for purely algebraic methods. The pseudo phase space formulation of quantum mechanics is self-contained. That is, there is no need, in principle, to switch to the Schroedinger or Heisenberg pictures when solving physical problems, although it may often be convenient to do so. The classical appearance of the pseudo phase space scheme is especially useful when considering the semi-classical limit of quantum mechanics. In fact, for potentials up to and including the harmonic oscillator the equations represent classical motion.

The structure of the thesis is such that it takes the reader steadily through the major concepts of pseudo phase space theory. The mathematical techniques that shall be needed are developed early in Chapter 1. These are used throughout the thesis. This presents the advantage that the reader is not faced with learning new mathematical methods as the thesis proceeds.

The pseudo phase space formulation of quantum mechanics as found applications in all areas of mathematical physics. Hence, there is a considerable amount of specialist literature available on the subject. It is hoped that this thesis serves as an introduction.

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CHAPTER ONE

THE WEYL CORRESPONDENCE RULE

1.1 INTRODUCTION.

Since the development of quantum mechanics one of the primary concerns has been its interface with classical Newtonian mechanics. In what was called the old quantum theory, Bohr introduced a correspondence principle as a way of using the classical theory as a limiting case to deduce some properties of atomic systems. In the wave formulation of quantum mechanics it has been an interesting exercise to ascertain that the theory reduces to the proper classical limit. This limit is understood (in its simplest form) to be the process of allowing \hbar (Planck's constant divided by 2π) to become zero. In nature \hbar is a non-zero constant and the classical limit can be taken to apply when \hbar is so small that for all intents and purposes it can be neglected, which is mathematically equivalent to letting \hbar become zero. However, care must be taken when this formal limit is administered since the quantities of interest often have singular behaviour in this limit.

In our case we are interested in how functions of the position and momentum operators are associated with their classical counterparts in phase space. The phase space to be discussed is referred to as "pseudo" or "mock" phase space. This is because phase space is a classical construct and so cannot exist in quantum mechanics. The objective of this thesis is to describe the formulation of quantum mechanics in pseudo phase space and, to some extent, look at implications for the classical limit. The origins of this formulation can be traced back to Weyl [7], Wigner [18] and Moyal [19]. One must also be aware of the fact that this formulation is completely quantum. It follows, therefore, that pseudo phase space must reduce to classical phase space when the limit is imposed that \hbar tends to zero. In fact, actual quantum calculations can usually be satisfactorily computed using the ordinary formalism of quantum mechanics. We are thus given the impression that pseudo phase space formulation is to some extent

aesthetic. However, its applicability becomes apparent when calculating quantum corrections to classical results when the corrections are small. We shall see later (cf Chapter 2) that Wigner invented his function to do just that for statistical mechanics. Even so, one is still at liberty to use the WKB expansion for Schroedinger's equation to calculate the semi-classical corrections.

The mathematical language of quantum mechanics is that of elements and operators in Hilbert space. Hilbert space is an infinite dimensional vector space spanned by vectors of complex functions of real variables, as opposed to the vectors spanning our familiar 3-dimensional Euclidean space. (Actually, since Hilbert and Euclidean vector spaces are complete, normed, vector spaces, they represent two examples of Banach spaces used in mathematical physics). Any devised correspondence rule is required to link the non-commuting quantum operators to commuting classical functions. There are various correspondence rules in existence, such as the von Neumann rule, Dirac rule, Born-Jordan rule, Riviers rule to name just a few [5,6]. The reason for the existence of several rules of association stems from the question of how to generate quantum operators from their classical counterparts. For example, take a product of the operators \hat{p} and \hat{q} . The correspondence rules, standard ordering, $\hat{q}\hat{p}$, anti-standard ordering, $\hat{p}\hat{q}$, and symmetric ordering, $(1/2)(\hat{q}\hat{p} + \hat{p}\hat{q})$, each produce the classical, commuting, product pq when \hat{p} and \hat{q} are replaced with their classical counterparts, [5]. Any sensible correspondence rule connecting quantum operators with phase space functions is perfectly valid. Each correspondence rule produces its own associated quasi-probability distribution functions in pseudo phase space. The prefix "quasi" is there to remind us that they are not true probability distributions owing to their ability to become negative (or even imaginary for some functions) in certain regions of pseudo phase space. Indeed, for practical work it is

often useful to opt for the simplest and if possible the most classical looking rule of association. The question of selecting the best pseudo phase space distribution function when investigating a particular physical phenomenon is at present unanswered, [6], but the choice of Weyl and Wigner is usually the simplest.

The rule of association that we shall therefore be chiefly interested in is the one given first by Weyl [7]. Whilst demonstrating the relationship existing between quantum mechanics and group theory he suggested a correspondence rule which produced a one-to-one mapping between quantum operators and classical functions. Due possibly to the group theory analogy, this rule did not appear to arouse much attention. It wasn't appreciably clear, until much later, how important Weyl's rule would be in the development of pseudo phase space formulation of quantum mechanics.

In this Chapter we shall investigate the main concepts of Weyl's rule of association and fix the nomenclature that will be used throughout this thesis. In so doing, we shall develop the basic mathematical tools that we shall need in our analysis of pseudo phase space. We shall not endeavour to cover the wide range of expressions that are available as these can be found in the literature. DeGroot and Suttorp, [1], provide in their book an encyclopaedic treatment of analysis in pseudo phase space, outlining numerous definitions and diverse expressions.

Incidentally, one may be wondering about the multiplicity of the expressions that we shall derive, or asking whether they are just for academic interest. Well, yes, they do contain a degree of academic interest. Probably, the most important reason for deriving them is, as we shall discover, that for particular calculation or derivation one definition can be far better to use than another. That is to say, one will arrive at a result quicker and (usually) easier when using one relation as opposed to another. The choice, of course, resides with the individual.

In Section 1.2 we formally establish the Weyl correspondence rule as it was originally proposed, [7], in terms of a Fourier integral. Some interesting expressions are derived in Section 1.3 which will a) enable us to invert and complete the Weyl correspondence by introducing the concept of the Weyl transform, and, b) provide useful results that will be essential for later chapters, [2,3]. Section 1.4 illustrates some of the main ideas with special cases. In Section 1.5 we show how to obtain Weyl transforms of simple functions without the need of integration, through the use of Bopp operators [8,9]. In Section 1.6 we investigate the relationship between the parity operator and a certain operator called the delta operator. Section 1.7 examines the displacement operator of Glauber, [13], and shows that it is a natural element of the Weyl correspondence rule. In Section 1.8 we analyse the symmetry properties of the Weyl transform and find that the displacement operator plays a central role in showing Galilean invariance. Finally, in Section 1.9 we generalise the main concepts of Weyl's rule through the use of symplectic notation. We then show that Weyl transforms of generalised products assume an elegant symplectic form.

1.2 MATHEMATICAL FORMULATION OF THE WEYL CORRESPONDENCE RULE

Weyl, [7], proposed a rule of association connecting quantum operators and classical functions by first writing a classical phase space function, $A^{cl}(pq)$, in its Fourier representation as[#]

$$A^{cl}(pq) = \int \alpha(u,v) \exp\left\{-\frac{i}{\hbar} [qu + pv]\right\} du dv$$

where $\alpha(u,v)$ is the Fourier transform of $A^{cl}(pq)$.

We shall generalise Weyl's proposal to functions on pseudo phase space. Thus, the Fourier integral of a pseudo phase space function, $A^w(pq)$, can be written as

$$A^w(pq) = \int \alpha(u,v) \exp\left\{-\frac{i}{\hbar} [qu + pv]\right\} du dv \quad (1.2.1)$$

Taking (with Weyl) for the process of quantisation the convention that p and q are replaced by their equivalent operator representatives, we get

$$\hat{A} = \int \alpha(u,v) \exp\left\{-\frac{i}{\hbar} [\hat{q}u + \hat{p}v]\right\} du dv \quad (1.2.2)$$

where \hat{A} is the operator associated with $A^w(pq)$.

[#] All limits of integration shall be assumed to extend from $-\infty$ to ∞ unless stated otherwise. For simplicity, we shall consider only one dimension although the transformation to higher dimensions is straightforward.

Eliminating $\alpha(u,v)$ from equations (1.2.1) and (1.2.2) gives Weyl's correspondence rule as

$$\hat{A} = \frac{1}{h} \int A^W(pq) \hat{\Delta}_{pq} dp dq \quad (1.2.3)$$

where the delta operator, $\hat{\Delta}_{pq}$, is given by

$$\hat{\Delta}_{pq} = \frac{1}{h} \int \exp\left\{\frac{i}{h} [(q - \hat{q})u + (p - \hat{p})v]\right\} du dv \quad (1.2.4)$$

and $A^W(pq)$ is called the Weyl transform of the operator \hat{A} .

Equation (1.2.3), in conjunction with (1.2.4), enables us to obtain the operator \hat{A} to be associated (in Weyl's scheme) with any function on pseudo phase space. However, this is only half of the Weyl correspondence. The picture is completed when we are able to find $A^W(pq)$ given \hat{A} . This is finalised below (cf equation (1.3.15)).

Weyl transforms are, in general, complex functions of real variables on pseudo phase space and thus $A^W(pq)$ is not identical to the classical phase space function $A^{cl}(pq)$. In addition, $A^W(pq)$ does not conform to the commuting algebra of classical functions (cf last 2 examples in Section 1.4). We have, therefore, an immediate contradiction with Weyl's original proposal [7]. Thus, as a cautionary note, one must not confuse the classical function $A^{cl}(pq)$ with the Weyl transform $A^W(pq)$. The former is obtained from the latter only when $\hbar \rightarrow 0$, or when the operator \hat{A} depends only on \hat{p} or \hat{q} , or sums of functions depending only on \hat{p} or upon \hat{q} .

1.3 INVERTING THE WEYL CORRESPONDENCE RULE

In the preceding Section we formally stated Weyls' rule, equation (1.2.3). It is the intention of this Section to extend our mathematical vocabulary in order to progress with some dexterity. Thus, we are going to derive some expressions, all stemming from equations (1.2.3) and (1.2.4), that will prove extremely useful in subsequent chapters.

Starting with equation (1.2.4) and applying the Baker - Campbell - Hausdorff Theorem, BCH Theorem [10]

$$\exp\{\hat{A} + \hat{B}\} = \exp\{\hat{A}\}\exp\{\hat{B}\}\exp\left\{-\frac{1}{2} [\hat{A}, \hat{B}]\right\} \quad (1.3.1)$$

which holds when $[\hat{A}, \hat{B}]$ commutes with both \hat{A} and \hat{B} .

We find that

$$\begin{aligned} \hat{\Delta}_{pq} &= \frac{1}{h} \int \exp\left\{\frac{i}{2h} uv\right\} \exp\left\{\frac{i}{h}(q - \hat{q})u\right\} \exp\left\{\frac{i}{h}(p - \hat{p})v\right\} dudv \\ &= \frac{1}{h} \int \exp\left\{-\frac{i}{2h} uv\right\} \exp\left\{\frac{i}{h}(p - \hat{p})v\right\} \exp\left\{\frac{i}{h}(q - \hat{q})u\right\} dudv \\ &= \int \exp\left\{\frac{i}{h}(p - \hat{p})v\right\} \delta\left(q - \frac{v}{2} - \hat{q}\right) dv \end{aligned} \quad (1.3.2)$$

where we have used the definition

$$\delta(x - a) = \frac{1}{2\pi} \int \exp\{i(x - a)y\} dy \quad (1.3.3)$$

for the Dirac δ - function to obtain equation (1.3.2).

We know from ordinary quantum mechanics, [11], that the projection operator is equivalent to the δ - function, ie,

$$\delta(q - \hat{q})|q'\rangle = |q\rangle\langle q|q'\rangle \quad (1.3.4)$$

hence equation (1.3.2) becomes

$$\hat{\Delta}_{pq} = \int \exp\left\{\frac{i}{\hbar}(p - \hat{p})v\right\} |q - \frac{v}{2}\rangle\langle q - \frac{v}{2}| dv \quad (1.3.5)$$

Furthermore, we know that

$$\exp\left\{-\frac{i}{\hbar} \hat{p}v\right\} |q\rangle = |q + v\rangle \quad (1.3.6)$$

and we finally get

$$\hat{\Delta}_{pq} = \int \exp\left\{\frac{i}{\hbar}pv\right\} |q + \frac{v}{2}\rangle\langle q - \frac{v}{2}| dv \quad (1.3.7)$$

It is quite straightforward to express $\hat{\Delta}_{pq}$ in terms of momentum eigenstates as

$$\hat{\Delta}_{pq} = \int \exp\left\{\frac{i}{\hbar}qu\right\} |p - \frac{u}{2}\rangle\langle p + \frac{u}{2}| du \quad (1.3.8)$$

Where we have used

$$\langle q|p\rangle = \frac{1}{\sqrt{h}} \exp\left\{\frac{i}{h}pq\right\} \quad (1.3.9)$$

so that

$$\int |p\rangle\langle p| dp = 1 = \int |q\rangle\langle q| dq \quad (1.3.10)$$

In addition, we know, [11], that the projection operator forms a complete basis for an arbitrary Hilbert space vector. That is, an arbitrary state vector $|\alpha\rangle$ can be expanded as

$$|\alpha\rangle = \sum_n |n\rangle\langle n|\alpha\rangle \quad (1.3.11)$$

From equations (1.3.7) and (1.3.8) we have

$$\frac{1}{h} \int \hat{\Delta}_{pq} dp = |q\rangle\langle q| \quad (1.3.12a)$$

and

$$\frac{1}{h} \int \hat{\Delta}_{pq} dq = |p\rangle\langle p| \quad (1.3.12b)$$

Hence, we see that $\hat{\Delta}_{pq}$ forms a complete basis for the set of linear operators.

Integrating equation (1.3.12a) over q or equation (1.3.12b) over p and using the closure relations (1.3.10) yields

$$\frac{1}{h} \int \hat{\Delta}_{pq} dp dq = 1 \quad (1.3.13)$$

Taking the trace of the product of equations (1.3.7) and (1.3.8) we have

$$\text{Tr}[\hat{\Delta}_{pq} \hat{\Delta}_{p',q'}] = h \delta(p - p') \delta(q - q') \quad (1.3.14)$$

where Tr stands for the trace.

Multiplying both sides of equation (1.2.3) by $\hat{\Delta}_{p',q'}$, taking the trace and using equation (1.3.14) enables us to write the Weyl transform in a more succinct form as

$$A^W(pq) = \text{Tr}[\hat{A} \hat{\Delta}_{pq}] \quad (1.3.15)$$

Equation (1.3.15) completes, with equation (1.2.3), the Weyl correspondence between functions on pseudo phase space and operators. Taking both equations (1.2.3) and (1.3.15) it is clear that Weyls' correspondence rule is indeed a one-to-one mapping between quantum operators and functions on pseudo phase space.

Substituting equation (1.3.7) into (1.3.15) gives an alternative form of Weyls' transform as

$$A^W(pq) = \int \exp\left\{\frac{i}{h} p v\right\} \langle q - \frac{v}{2} | \hat{A} | q + \frac{v}{2} \rangle dv \quad (1.3.16)$$

From equation (1.3.16), it is apparent that $A^W(pq)$ is real if \hat{A} is an

Hermitian operator.

The Weyl transform of the product $\hat{A}\hat{B}$ is not, in general, simply $A^W(pq)B^W(pq)$ but is rather more complicated. The procedure for finding the Weyl transform of the product $\hat{A}\hat{B}$ is as follows. From equation (1.2.3) we get

$$\hat{A}\hat{B} = \frac{1}{h^2} \int A^W(pq) B^W(p'q') \hat{\Delta}_{pq} \hat{\Delta}_{p'q'} dp dq dp' dq' \quad (1.3.17)$$

using equation (1.2.4) for the delta operators and applying the BCH Theorem, equation (1.3.1), to the product $\hat{\Delta}_{pq} \hat{\Delta}_{p'q'}$ we have

$$\begin{aligned} \hat{\Delta}_{pq} \hat{\Delta}_{p'q'} = \frac{1}{h^2} \int \exp \left\{ -\frac{i}{2h} [uv' - vu'] \right\} \exp \left\{ \frac{i}{h} \left[(q - \hat{q})u + (p - \hat{p})v \right. \right. \\ \left. \left. + (q' - \hat{q}')u' + (p' - \hat{p}')v' \right] \right\} du dv du' dv' \end{aligned}$$

and replacing

$$uv' \text{ by } -\hbar^2 \frac{\partial^2}{\partial p' \partial q} \quad \text{and } vu' \text{ by } -\hbar^2 \frac{\partial^2}{\partial p \partial q'}$$

we get,

$$\begin{aligned} \hat{\Delta}_{pq} \hat{\Delta}_{p'q'} = \frac{1}{h^2} \int \exp \left\{ \frac{i\hbar}{2} \left[\frac{\partial^2}{\partial q \partial p'} - \frac{\partial^2}{\partial p \partial q'} \right] \right\} \exp \left\{ \frac{i}{h} \left[-\hat{q}(u + u') \right. \right. \\ \left. \left. - \hat{p}(v + v') + qu + q'u' + pv + p'v' \right] \right\} du dv du' dv' \end{aligned}$$

Transform the variables according to the rule,

$$u = u'' + \frac{u' ''}{2}, \quad u' = -u'' + \frac{u' ''}{2}, \quad v = v'' + \frac{v' ''}{2}, \quad v' = -v'' + \frac{v' ''}{2}$$

and using equation (1.3.3) we have

$$\hat{\Delta}_{pq} \hat{\Delta}_{p',q'} = \text{hexp} \left\{ \frac{i\hbar}{2} \left[\frac{\partial^2}{\partial q \partial p'} - \frac{\partial^2}{\partial p \partial q'} \right] \right\} \delta(p - p') \delta(q - q') \hat{\Delta}_{pq} \quad (1.3.18)$$

Inserting equation (1.3.18) into (1.3.17) and following a partial integration

$$\hat{A}\hat{B} = \frac{1}{h} \int A^W(pq) \exp \left\{ \frac{i\hbar}{2} \left[\overset{\leftarrow}{\partial} \overset{\rightarrow}{\partial} \frac{\partial}{\partial q \partial p} - \overset{\leftarrow}{\partial} \overset{\rightarrow}{\partial} \frac{\partial}{\partial p \partial q} \right] \right\} B^W(pq) \hat{\Delta}_{pq} dp dq$$

The arrows indicate on which function the exponential operator acts. This notation shall be adopted throughout the thesis. Multiplying both sides by $\hat{\Delta}_{p',q'}$, taking the trace and using equation (1.3.14), or, by comparing directly with equation (1.2.3) we finally get for the Weyl transform of $\hat{A}\hat{B}$

$$[\hat{A}\hat{B}]_{pq}^W = A^W(pq) \exp \left\{ \frac{i\hbar}{2} \left[\overset{\leftarrow}{\partial} \overset{\rightarrow}{\partial} \frac{\partial}{\partial q \partial p} - \overset{\leftarrow}{\partial} \overset{\rightarrow}{\partial} \frac{\partial}{\partial p \partial q} \right] \right\} B^W(pq) \quad (1.3.19)$$

where we have introduced the notation $[\hat{A}\hat{B}]_{pq}^W$ on the lhs of equation (1.3.19). This signifies that we must take the Weyl transform of the resulting operator within the square brackets.

An alternative expression for $[\hat{A}\hat{B}]_{pq}^W$, due to Groenewold [2,4], can be found by expanding the exponential operator in equation (1.3.19) to get

$$\begin{aligned}
[\hat{A}\hat{B}]_{pq}^W &= A^W(pq) \left[\sum \frac{1}{n!} \left[\frac{i\hbar}{2} \right]^n \left[\frac{\overset{\leftarrow}{\partial} \overset{\rightarrow}{\partial}}{\partial q \partial p} - \frac{\overset{\leftarrow}{\partial} \overset{\rightarrow}{\partial}}{\partial p \partial q} \right]^n \right] B^W(pq) \\
&= A^W \left[p - \frac{i\hbar}{2} \frac{\partial}{\partial q}, q + \frac{i\hbar}{2} \frac{\partial}{\partial p} \right] B^W(pq) \\
&= B^W \left[p + \frac{i\hbar}{2} \frac{\partial}{\partial q}, q - \frac{i\hbar}{2} \frac{\partial}{\partial p} \right] A^W(pq) \tag{1.3.20}
\end{aligned}$$

There are two more results that will prove useful later on. These, again, can be obtained directly from equation (1.2.3). They are, first,

$$\text{Tr}[\hat{A}] = \frac{1}{h} \int A^W(pq) dp dq \tag{1.3.21}$$

where we have used the result $\text{Tr}[\hat{\Delta}_{pq}] = 1$, and, second,

$$\text{Tr}[\hat{A}\hat{B}] = \frac{1}{h} \int A^W(pq) B^W(pq) dp dq \tag{1.3.22}$$

where we have used equations (1.2.3) and (1.3.14) in the derivation.

1.4 SPECIAL CASES OF THE WEYL CORRESPONDENCE RULE

In this Section we shall generate, for completeness as opposed to being pedantic, a short list of special instances of the Weyl correspondence, equations (1.2.3) and (1.3.15). The two way arrows infer the one-to-one relationship shared by the quantum operators and their associated Weyl transforms.

$$1 \rightleftharpoons 1$$

$$f(\hat{p}) \rightleftharpoons f(p)$$

$$g(\hat{q}) \rightleftharpoons g(q)$$

$$\hat{p}\hat{q} \rightleftharpoons pq - \frac{i\hbar}{2}$$

$$\hat{q}\hat{p} \rightleftharpoons pq + \frac{i\hbar}{2}$$

An inspection of these mappings reveals some interesting features borne out of the Weyl correspondence rule. In fact, simple as they are, they serve to be both instructive and provide examples of complex pseudo phase space functions. Incidentally, from the last two correspondences we find that the commutation rule $[\hat{p}, \hat{q}] = -i\hbar$ holds true.

1.5 BOPP OPERATORS AND THE WEYL TRANSFORM

So far we have concerned ourselves with operators in Hilbert space. In this Section we shall define two very interesting operators, called Bopp operators [8,9]. Applying these operators to our Hilbert space operators we shall create new operators on pseudo phase space. Consequently, these pseudo phase space operators will enable us to calculate Weyl transforms without the need to integrate. However, the drawback with this method is that it can only be used with ease for simple cases. (All the examples stipulated in the previous Section follow quickly by this technique, but it gets complicated for less simple cases).

By definition, we have

$$\begin{aligned} A^B(pq) &\equiv \hat{A} \\ \hat{p} &\rightarrow p^B \\ \hat{q} &\rightarrow q^B \end{aligned}$$

and

$$\begin{aligned} \Delta^B(pq;p'q') &= \hat{\Delta}_{pq} \\ \hat{p} &\rightarrow p'^B \\ \hat{q} &\rightarrow q'^B \end{aligned}$$

where

$$p^B = p - \frac{i\hbar}{2} \frac{\partial}{\partial q}, \quad q^B = q + \frac{i\hbar}{2} \frac{\partial}{\partial p} \quad (1.5.1)$$

and

$$p'^B = p' - \frac{i\hbar}{2} \frac{\partial}{\partial q'}, \quad q'^B = q' + \frac{i\hbar}{2} \frac{\partial}{\partial p'} \quad (1.5.2)$$

are the Bopp operators.

Before proceeding it will be useful to apply the BCH Theorem, equation (1.3.1), to equation (1.2.4) to get

$$\hat{\Delta}_{pq} = \frac{1}{\hbar} \int \exp\left\{\frac{i}{\hbar}(qu + pv)\right\} \exp\left\{\frac{i}{2\hbar} uv\right\} \exp\left\{-\frac{i}{\hbar} \hat{q}u\right\} \exp\left\{-\frac{i}{\hbar} \hat{p}v\right\} du dv \quad (1.5.3)$$

The application of the Bopp operators in finding Weyl transforms of operators can be shown by substituting equation (1.5.2) into (1.5.3). Let the resulting operator act on a constant, say 1, to get

$$\begin{aligned} \Delta^B(pq; p'q') * 1 &= \frac{1}{\hbar} \int \exp\left\{\frac{i}{\hbar}(qu + pv)\right\} \exp\left\{\frac{i}{2\hbar} uv\right\} \\ &\times \exp\left\{-\frac{i}{\hbar}\left(q' + \frac{i\hbar}{2} \frac{\partial}{\partial p'}\right)u\right\} \exp\left\{-\frac{i}{\hbar}\left(p' - \frac{i\hbar}{2} \frac{\partial}{\partial q'}\right)v\right\} du dv * 1 \\ &= \frac{1}{\hbar} \int \exp\left\{\frac{i}{\hbar}(qu + pv)\right\} \exp\left\{\frac{i}{2\hbar} uv\right\} \exp\left\{-\frac{i}{\hbar}\left(q' + \frac{i\hbar}{2} \frac{\partial}{\partial p'}\right)u\right\} \\ &\times \exp\left\{-\frac{i}{\hbar} p'v\right\} du dv \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{h} \int \exp\left\{\frac{i}{h}(qu + pv)\right\} \exp\left\{\frac{i}{2h}uv\right\} \exp\left\{-\frac{i}{h}q'u\right\} \\
&\quad \times \exp\left\{-\frac{i}{h}\left(p' + \frac{u}{2}\right)v\right\} dudv \\
&= \frac{1}{h} \int \exp\left\{\frac{i}{h}\left[(q - q')u + (p - p')v\right]\right\} dudv \\
&= h \delta(q - q') \delta(p - p') \tag{1.5.4}
\end{aligned}$$

Substituting equation (1.5.4) into (1.2.3) and carrying out the integration gives

$$A^B(pq) * 1 = A^W(pq) \tag{1.5.5}$$

Equation (1.5.5) states that for any operator written as a function of \hat{p} and \hat{q} one must replace these operators by their Bopp equivalents. Then applying the resulting operator to 1 gives the Weyl transform of the original operator. What is most interesting and appealing about this method is that there is no need to do any integrals.

For example, we shall find the Weyl transform of the product $\hat{p}\hat{q}$ by using the above prescription. We first replace the product with their corresponding Bopp operators and operate on 1, thus

$$\hat{p}\hat{q} \begin{matrix} \longrightarrow \\ \longleftarrow \end{matrix} \left[p - \frac{i\hbar}{2} \frac{\partial}{\partial q}\right] \left[q + \frac{i\hbar}{2} \frac{\partial}{\partial p}\right] * 1 = pq - \frac{i\hbar}{2} \tag{1.5.6}$$

and similarly for $\hat{q}\hat{p}$, gives

$$\hat{q}\hat{p} \xrightarrow{\leftarrow} \left[q + \frac{i\hbar}{2} \frac{\partial}{\partial p} \right] \left[p - \frac{i\hbar}{2} \frac{\partial}{\partial q} \right] * 1 = pq + \frac{i\hbar}{2} \quad (1.5.7)$$

Equations (1.5.6) and (1.5.7) can be compared with the last two special cases in Section 1.4.

Clearly, the Bopp operators, being operators in pseudo phase space, satisfy the commutation relation

$$\left[\left\{ p - \frac{i\hbar}{2} \frac{\partial}{\partial q} \right\}, \left\{ q + \frac{i\hbar}{2} \frac{\partial}{\partial p} \right\} \right] = -i\hbar \quad (1.5.8)$$

To gain further insight into this technique we shall derive equation (1.3.19), the Weyl transform of a product of operators.

We shall begin with

$$[\hat{A}\hat{B}]_{pq}^w = [\hat{A}\hat{B}]_{pq}^B * 1 \quad (1.5.9)$$

and using equation (1.5.5) we have immediately

$$\begin{aligned} [\hat{A}\hat{B}]_{pq}^w &= [\hat{A}\hat{B}]_{pq}^B * 1 \\ &= A^B(pq) B^B(pq) * 1 \\ &= A^B(pq) * B^w(pq) \end{aligned} \quad (1.5.10)$$

From equation (1.2.3) and the definition of $A^B(pq)$, equation (1.5.10) becomes

$$[\hat{A}\hat{B}]_{pq}^w = \frac{1}{h} \int A^w(p'q') [\Delta^B(p'q';pq) * B^w(pq)] dp' dq' \quad (1.5.11)$$

The bracketed term in equation (1.5.11) can be evaluated by using equation (1.5.3), to get

$$\begin{aligned} \Delta^B(pq;p'q') * B^w(pq) &= \frac{1}{h} \int \exp\left\{\frac{i}{h}(qu + pv)\right\} \exp\left\{\frac{i}{2h} uv\right\} \\ &\times \exp\left\{-\frac{i}{h}\left[q' + \frac{i\hbar}{2} \frac{\partial}{\partial p'}\right]u\right\} \exp\left\{-\frac{i}{h}\left[p' - \frac{i\hbar}{2} \frac{\partial}{\partial q'}\right]v\right\} B^w(p'q') du dv \\ &= \frac{1}{h} \int \exp\left\{\frac{i}{h}(qu + pv)\right\} \exp\left\{\frac{i}{2h} uv\right\} \exp\left\{-\frac{i}{h}\left[q' + \frac{i\hbar}{2} \frac{\partial}{\partial p'}\right]u\right\} \\ &\times \exp\left\{-\frac{i}{h} p' v\right\} B^w(p', q' - \frac{v}{2}) du dv \\ &= \frac{1}{h} \int \exp\left\{\frac{i}{h}(qu + pv)\right\} \exp\left\{\frac{i}{2h} uv\right\} \exp\left\{-\frac{i}{h} q' u\right\} \\ &\times \exp\left\{-\frac{i}{h}\left(p' + \frac{u}{2}\right)v\right\} B^w\left(p' + \frac{u}{2}, q' - \frac{v}{2}\right) du dv \\ &= \frac{1}{h} \int \exp\left\{\frac{i}{h}(qu + pv)\right\} \exp\left\{-\frac{i}{h}\left[q' + \frac{i\hbar}{2} \frac{\partial}{\partial p'}\right]u\right\} \\ &\times \exp\left\{-\frac{i}{h}\left[p' - \frac{i\hbar}{2} \frac{\partial}{\partial q'}\right]v\right\} B^w(p'q') du dv \end{aligned}$$

Here the arrows indicate that the differential operators act only on $B^W(p'q')$. We have

$$\begin{aligned}
\Delta^B(pq; p'q') &= \frac{1}{\hbar} \int \exp\left\{\frac{i}{\hbar}(qu + pv)\right\} \exp\left\{-\frac{i}{\hbar}(q'u + p'v)\right\} \\
&\quad \times \exp\left\{\left[\frac{u}{2} \frac{\partial}{\partial p'} - \frac{v}{2} \frac{\partial}{\partial q'}\right]\right\} B^W(p'q') du dv \\
&= \frac{1}{\hbar} \int \exp\left\{\frac{i}{\hbar}[(q - q')u + (p - p')v]\right\} \exp\left\{\frac{i\hbar}{2}\left[\frac{\overleftarrow{\partial}}{\partial q' \partial p'} - \frac{\overrightarrow{\partial}}{\partial p' \partial q'}\right]\right\} \\
&\quad \times B^W(p'q') du dv \quad (1.5.12)
\end{aligned}$$

where we have replaced

$$u \text{ by } -\frac{\hbar}{i} \frac{\overleftarrow{\partial}}{\partial q'}, \quad \text{and} \quad v \text{ by } -\frac{\hbar}{i} \frac{\overleftarrow{\partial}}{\partial p'},$$

to get equation (1.5.12).

Substituting equation (1.5.12) into (1.5.11) yields the final result as follows

$$\begin{aligned}
(\hat{A}\hat{B})_{pq}^B * 1 &= (\hat{A}\hat{B})_{pq}^W = \frac{1}{\hbar^2} \int A^W(pq) \exp\left\{\frac{i}{\hbar}[(q - q')u + (p - p')v]\right\} \\
&\quad \times \exp\left\{\frac{i\hbar}{2}\left[\frac{\overleftarrow{\partial}}{\partial q' \partial p'} - \frac{\overrightarrow{\partial}}{\partial p' \partial q'}\right]\right\} B^W(p'q') dp dq du dv
\end{aligned}$$

$$\begin{aligned}
&= \int A^W(pq) \delta(q - q') \delta(p - p') \\
&\quad \times \exp \left\{ \frac{i\hbar}{2} \left[\frac{\overleftarrow{\partial}}{\partial q'} \frac{\overrightarrow{\partial}}{\partial p'} - \frac{\overleftarrow{\partial}}{\partial p'} \frac{\overrightarrow{\partial}}{\partial q'} \right] \right\} B^W(p'q') dp dq \\
&= A^W(pq) \exp \left\{ \frac{i\hbar}{2} \left[\frac{\overleftarrow{\partial}}{\partial q} \frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p} \frac{\overrightarrow{\partial}}{\partial q} \right] \right\} B^W(pq) \quad (1.5.13)
\end{aligned}$$

As an example of the application of the Bopp operators we shall find the Weyl transform of $\hat{\Delta}_{pq}$.

We apply the BCH Theorem, equation (1.3.1), to equation (1.2.4) to get

$$\hat{\Delta}_{pq} = \frac{1}{\hbar} \int \exp \left\{ \frac{i\hbar}{2} uv \right\} \exp \left\{ \frac{i}{\hbar} (pv + qu) \right\} \exp \left\{ -\frac{i}{\hbar} \hat{p}v \right\} \exp \left\{ -\frac{i}{\hbar} \hat{q}u \right\} du dv \quad (1.5.14)$$

Inserting the Bopp operators, equation (1.5.2), in equation (1.5.14) gives

$$\begin{aligned}
[\hat{\Delta}_{pq}]_{pq}^W &= \frac{1}{\hbar} \int \exp \left\{ \frac{i\hbar}{2} \frac{\partial^2}{\partial p \partial q} \right\} \exp \left\{ \frac{i}{\hbar} (pv + qu) \right\} \\
&\quad \times \exp \left\{ -\frac{i}{\hbar} \left[p' - \frac{i\hbar}{2} \frac{\partial}{\partial q'} \right] \right\} \exp \left\{ -\frac{i}{\hbar} \left[q' + \frac{i\hbar}{2} \frac{\partial}{\partial p'} \right] \right\} du dv * 1 \\
&= \frac{1}{\hbar} \int \exp \left\{ \frac{i\hbar}{2} \frac{\partial^2}{\partial p \partial q} \right\} \exp \left\{ \frac{i}{\hbar} (pv + qu) \right\} \exp \left\{ -\frac{i}{\hbar} p'v \right\} \\
&\quad \times \exp \left\{ -\frac{i}{\hbar} (q' - \frac{1}{2} uv) \right\} du dv
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{h} \int \exp\left\{\frac{i\hbar}{2} \frac{\partial^2}{\partial p \partial q}\right\} \exp\left\{-\frac{i\hbar}{2} \frac{\partial^2}{\partial p \partial q}\right\} \\
&\quad \times \exp\left\{\frac{i}{\hbar}[(p - p')v + (q - q')u]\right\} du dv \\
&= h \delta(p - p') \delta(q - q') \tag{1.5.15}
\end{aligned}$$

In practice one would use a more direct method in obtaining equation (1.5.15) by combining equations (1.3.14) and (1.3.15).

To summarise, the Bopp operators can prove to be a very useful tool for obtaining Weyl transforms of quantum operators. This is a result of the integrals being replaced by differential operators which are (sometimes) easier to evaluate. However, as previously mentioned, they can only be used with confidence in simple applications.

1.6 PARITY AND THE WEYL TRANSFORM

The energy eigenfunctions, for symmetric potentials, can either be symmetric or anti-symmetric functions of the co-ordinates in configuration space. In ordinary quantum mechanics, [11], this symmetry property is referred to as parity. For such potentials eigenfunctions have either even (symmetric) or odd (anti-symmetric) parity. The parity operator, $\hat{\Pi}$, which changes the signs of the co-ordinates is defined by

$$\hat{\Pi}\psi(x) \equiv \psi(-x) \tag{1.6.1}$$

The identity transformation follows from definition (1.6.1) as

$$\hat{\Pi}^2 \psi(x) = \psi(x) \quad (1.6.2)$$

From equation (1.6.2) we can deduce that for eigenfunctions with a definite parity, the eigenvalues of $\hat{\Pi}$ are ± 1 . The plus and minus signs indicate even and odd parity.

If an eigenfunction does not have a definite parity then (following [11]) it can be decomposed into a linear independent combination of even and odd eigenfunctions, that is

$$\psi(x) = \frac{1}{2} \left[\{ \psi(x) + \psi(-x) \} + \{ \psi(x) - \psi(-x) \} \right] \quad (1.6.3)$$

The parity of a state is a constant of motion in time if

$$[\hat{H}, \hat{\Pi}] = 0 \quad (1.6.4)$$

which is true if and only if the potential is symmetric. (Of course, this is not true for beta decay).

The $\hat{\Delta}_{pq}$ operator occurs naturally in the Weyl formalism and plays a central role within the Weyl transform theory. There exists a connection between $\hat{\Delta}_{pq}$ and $\hat{\Pi}$ which gives a possible physical interpretation of $\hat{\Delta}_{pq}$.

If $f(\hat{q} - q)$ is an arbitrary function that can be expanded in a power series, then by using equation (1.3.7) we have

$$\left(\frac{1}{2} \hat{\Delta}_{pq}\right) f(\hat{q} - q) \left(\frac{1}{2} \hat{\Delta}_{pq}\right) = f(q - \hat{q}) \quad (1.6.5)$$

In a similar fashion we have

$$(\frac{1}{2} \hat{\Delta}_{pq})g(\hat{p} - p)(\frac{1}{2} \hat{\Delta}_{pq}) = g(p - \hat{p}) \quad (1.6.6)$$

where we have used equation (1.3.8).

From equations (1.6.5) and (1.6.6) we see that $(1/2)\hat{\Delta}_{pq}$ reflects the pseudo phase points about p, q . If, for instance, we set $f(\hat{q} - q) = \hat{1}$ in equation (1.6.5) then

$$(\frac{1}{2} \hat{\Delta}_{pq})^2 = 1 \quad (1.6.7)$$

In general we can show that

$$(\frac{1}{2} \hat{\Delta}_{pq})F(\hat{p} - p, \hat{q} - q)(\frac{1}{2} \hat{\Delta}_{pq}) = F(p - \hat{p}, q - \hat{q}) \quad (1.6.8)$$

By combining equations (1.6.7) and (1.6.8) we can define

$$\hat{\Pi}_{pq} \equiv \frac{1}{2} \hat{\Delta}_{pq} \quad (1.6.9)$$

where $\hat{\Pi}_{pq}$ is the pseudo phase space parity operator, [12].

The Weyl transform of $\hat{\Pi}_{pq}$ is effected by applying equations (1.3.14) and (1.3.15) to definition (1.6.9), namely

$$[\hat{\Pi}_{p',q'}]_{pq}^w = \text{Tr}[\hat{\Pi}_{p',q'} \hat{\Delta}_{pq}]$$

$$= \frac{\hbar}{2} \delta(p - p') \delta(q - q') \quad (1.6.10)$$

The Weyl transform of the parity operator $\hat{\Pi}$ is, by equation (1.3.16)

$$\begin{aligned} [\hat{\Pi}]_{pq}^w &= \int \exp\left\{\frac{i}{\hbar} p v\right\} \left\langle q - \frac{1}{2} v \middle| \hat{\Pi} \middle| q + \frac{1}{2} v \right\rangle dv \\ &= \int \exp\left\{\frac{i}{\hbar} p v\right\} \left\langle q - \frac{1}{2} v \middle| -q - \frac{1}{2} v \right\rangle dv \\ &= \frac{\hbar}{2} \delta(p) \delta(q) \end{aligned} \quad (1.6.11)$$

Comparing equations (1.6.10) and (1.6.11) we have

$$\hat{\Pi} = \hat{\Pi}_{p'=q'=0} \quad (1.6.12)$$

which shows that the parity operator is just the pseudo phase space parity operator centred around the origin.

1.7 THE PSEUDO PHASE SPACE DISPLACEMENT OPERATOR

The displacement operator was first introduced into quantum mechanics by Glauber, [13], through an analysis of the quantized radiation field using coherent states. These coherent states, denoted by $|\alpha\rangle$, are defined in terms of a linear superposition of the number states $|n\rangle$ as

$$|\alpha\rangle = \exp\left\{-\frac{|\alpha|^2}{2}\right\} \sum_n \frac{(\alpha)^n}{(n!)^{1/2}} |n\rangle \quad (1.7.1)$$

where α is any complex number.

The coherent states are normalized to unity as can be seen directly from equation (1.7.1), so that

$$\langle\alpha|\alpha\rangle = 1 \quad (1.7.2)$$

but they are not orthogonal since

$$|\langle\alpha|\beta\rangle|^2 = \exp\{-|\alpha - \beta|^2\} \quad (1.7.3)$$

where β is any complex number different from α . Indeed, if we impose the condition

$$|\alpha - \beta| \gg 1 \quad (1.7.4)$$

then the states $|\alpha\rangle$ and $|\beta\rangle$ become approximately orthogonal.

Since the α 's are complex then the set of coherent states $|\alpha\rangle$ exceeds the set of the number states $|n\rangle$. As a consequence of this coherent states form an overcomplete set.

The harmonic oscillator plays an important role in quantum field theory and from this the concept of the creation and destruction operators are introduced. Thus, for the creation operator \hat{a}^+ operating on the number state $|n\rangle$ we have the property

$$\hat{a}^+|n\rangle = \sqrt{(n+1)}|n+1\rangle \quad (1.7.5)$$

and for the destruction operator \hat{a} , we have

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \quad (1.7.6)$$

\hat{a}^+ and \hat{a} are the Hermitian conjugates of each other and are given in terms of \hat{p} and \hat{q} by

$$\hat{a}^+ = \left[\frac{1}{2\hbar m\omega} \right]^{\frac{1}{2}} (m\omega\hat{q} - i\hat{p}) \quad (1.7.7)$$

and

$$\hat{a} = \left[\frac{1}{2\hbar m\omega} \right]^{\frac{1}{2}} (m\omega\hat{q} + i\hat{p}) \quad (1.7.8)$$

From equations (1.7.5) and (1.7.6) we have

$$\hat{a}\hat{a}^+|n\rangle = (n+1)|n\rangle \quad (1.7.9)$$

and

$$\hat{a}^+\hat{a}|n\rangle = n|n\rangle \quad (1.7.10)$$

Thus, by subtracting equation (1.7.10) from (1.7.9) we obtain the commutation rule

$$[\hat{a}, \hat{a}^+] = 1 \quad (1.7.11)$$

The operator product $\hat{a}^+\hat{a}$, of equation (1.7.10), is called the number operator, \hat{n} ; its eigenvalue is the number of particles n .

By iteration and induction of equation (1.7.5) one can readily show that the number state $|n\rangle$ can be expressed in terms of the creation operator, as

$$|n\rangle = \left[\frac{1}{n!} \right]^{\frac{1}{2}} (\hat{a}^+)^n |0\rangle \quad (1.7.12)$$

Substituting equation (1.7.12) into (1.7.1) gives

$$|\alpha\rangle = \exp\{\alpha\hat{a}^+ - \alpha^*\hat{a}\} |0\rangle \quad (1.7.13)$$

where we have used the BCH Theorem, equation (1.3.1).

The exponential operator acts as the creation operator for coherent states; it is the displacement operator obtained by Glauber, [13]. Therefore, we shall define the displacement operator as

$$\begin{aligned} \hat{D}_\alpha &\equiv \exp\{\alpha\hat{a}^+ - \alpha^*\hat{a}\} \\ &= \exp\left\{-\frac{|\alpha|^2}{2}\right\} \exp\{\alpha\hat{a}^+\} \exp\{-\alpha^*\hat{a}\} \end{aligned} \quad (1.7.15)$$

To show the displacement property of equation (1.7.15) we shall need the following results

$$[\hat{a}, (\hat{a}^+)^n] = n(\hat{a}^+)^{n-1} \quad (1.7.16a)$$

$$[\hat{a}^+, \hat{a}^n] = -n\hat{a}^{n-1} \quad (1.7.16b)$$

$$\hat{D}_\alpha^+ = \exp\left\{\frac{|\alpha|^2}{2}\right\} \exp\{\alpha^* \hat{a}\} \exp\{-\alpha \hat{a}^+\} \quad (1.7.16c)$$

From which one easily finds

$$\hat{D}_\alpha^+ \hat{a} \hat{D}_\alpha = \hat{a} + \alpha \quad (1.7.17a)$$

$$\hat{D}_\alpha^+ \hat{a}^+ \hat{D}_\alpha = \hat{a}^+ + \alpha^* \quad (1.7.17b)$$

Substituting equation (1.7.7), (1.7.8) into (1.7.15) and noticing that the coefficient of \hat{p} has units of length and that of \hat{q} has units of momentum we can define the pseudo phase space displacement operator as

$$\begin{aligned} \hat{D}_{pq} &\equiv \exp\left\{\frac{i}{\hbar}(\hat{p}q + \hat{q}p)\right\} \\ &= \exp\left\{-\frac{i\hbar}{2}pq\right\} \exp\{\hat{p}q\} \exp\{\hat{q}p\} \end{aligned} \quad (1.7.18)$$

where we have used the BCH Theorem, equation (1.3.1).

It is easily seen that \hat{D}_{pq} satisfies the unitary condition

$$\hat{D}_{pq} \hat{D}_{pq}^+ = \hat{D}_{pq}^+ \hat{D}_{pq} = 1 \quad (1.7.19)$$

From equation (1.2.4), \hat{D}_{pq} arises naturally out of the Weyl correspondence as being the Fourier inverse of $\hat{\Delta}_{pq}$, that is

$$\hat{D}_{pq} = \frac{1}{h} \int \exp\left\{\frac{i}{h}(p'q + q'p)\right\} \hat{\Delta}_{p'q'} dp' dq' \quad (1.7.20)$$

An interesting property of the displacement operator follows directly from definition (1.7.18) and equation (1.3.1) as

$$\hat{D}_{p_1 q_1} \hat{D}_{p_2 q_2} = \exp\left\{\frac{i}{2h}(p_1 q_2 - q_1 p_2)\right\} \hat{D}_{p_1 + p_2, q_1 + q_2} \quad (1.7.21)$$

An important special case of equation (1.7.21) is obtained by setting $p_1 = p_2$ and $q_1 = q_2$ to get

$$\hat{D}_{pq} \hat{D}_{pq} = \hat{D}_{2p 2q} \quad (1.7.22)$$

We know from equation (1.6.12) that the pseudo phase space parity operator $\hat{\Pi}_{pq}$ is the displaced parity operator $\hat{\Pi}$. Following [12] and using equation (1.7.18) we have

$$\begin{aligned} \hat{D}_{pq}^\dagger \hat{\Pi}_{pq} \hat{D}_{pq} &= \int \exp\left\{\frac{i}{h} \hat{p} q\right\} \exp\left\{\frac{i}{h} \hat{q} p\right\} |v\rangle \langle -v| \left[\exp\left\{\frac{i}{h} \hat{p} q\right\} \exp\left\{\frac{i}{h} \hat{q} p\right\} \right]^\dagger dv \\ &= \int \exp\left\{\frac{2ipv}{h}\right\} |q + v\rangle \langle q - v| dv \end{aligned}$$

$$= \frac{1}{2} \hat{\Delta}_{pq}$$

$$= \hat{\Pi}_{pq} \quad (1.7.23)$$

where we have used equations (1.3.7) and (1.6.9).

Using the above result we are able to write down some alternative expressions for the Weyl transform of an arbitrary operator \hat{A} . Thus, from the defining equation (1.3.15) we have

$$A^W(pq) = 2\text{Tr} [\hat{A} \hat{\Pi}_{pq}] \quad (1.7.24a)$$

$$= 2\text{Tr} [\hat{A} \hat{D}_{pq} \hat{\Pi} \hat{D}_{pq}^+] \quad (1.7.24b)$$

In the next Section we shall discuss a further use of the pseudo phase space displacement operator.

1.8 SYMMETRIES OF THE WEYL TRANSFORM

The Weyl correspondence rule has been described only for systems in the non-relativistic limit. It is, therefore, natural for Weyls' rule to exhibit Galilean invariance. By Galilean invariance, we mean that for a closed system the equations are formally the same under the Galilean group of transformations. So that, if \hat{A} is transformed into \hat{A}' by a unitary transformation and the pseudo phase space co-ordinates p, q into p', q' then

the corresponding Weyl transforms of \hat{A} and \hat{A}' are related by

$$A^W(pq) = A'^W(p'q') \quad (1.8.1)$$

Equation (1.8.1) can be shown by utilising the displacement operator.

The Galilean transformation between two inertial frames S and S' , where S' moves with velocity V relative to S is given by

$$\begin{aligned} p' &= p - mV \\ q' &= q + q_0 - Vt \\ t' &= t \end{aligned} \quad (1.8.2)$$

where m is the mass, V the relative velocity, t the time and q_0 is a translation in position.

The displacement operator associated with the Galilean transformation is, from equation (1.7.18),

$$\hat{D}_{-mV, q_0 - Vt} = \exp \left\{ \frac{i}{\hbar} [\hat{p}(q_0 - Vt) - \hat{q}mV] \right\} \quad (1.8.3)$$

By definition of the Weyl transform, equation (1.3.15), we have

$$\begin{aligned} A^W(pq) &= \text{Tr} [\hat{A} \hat{\Delta}_{pq}] \\ &= \text{Tr} [\hat{D} \hat{A} \hat{D}^\dagger \hat{\Delta}_{pq} \hat{D}^\dagger] \end{aligned}$$

$$= \text{Tr} [\hat{A}' \hat{\Delta}_{p', q'}]$$

$$= A'^W(p', q') \quad (1.8.4)$$

where, using equations (1.3.1), (1.3.7) and (1.8.2), we have

$$\begin{aligned} \hat{\Delta}_{p', q'} &= \hat{D} \hat{\Delta}_{pq} \hat{D}^+ \\ &= \int \exp \left\{ \frac{i}{\hbar} p v \right\} \exp \left\{ \frac{i}{\hbar} \left[(q_0 - Vt) \hat{p} - mV \hat{q} \right] \right\} |q + \frac{1}{2} v \rangle \langle q - \frac{1}{2} v| \\ &\quad \times \left[\exp \left\{ \frac{i}{\hbar} \left[(q_0 - Vt) \hat{p} - mV \hat{q} \right] \right\} \right]^+ dv \\ &= \int \exp \left\{ \frac{i}{\hbar} (p - mV) v \right\} | (q + q_0 - Vt) + \frac{1}{2} v \rangle \\ &\quad \times \langle (q + q_0 - Vt) - \frac{1}{2} v | dv \\ &= \int \exp \left\{ \frac{i}{\hbar} p' v \right\} |q' + \frac{1}{2} v \rangle \langle q' - \frac{1}{2} v | dv \end{aligned} \quad (1.8.5)$$

Notice that the mathematical form of the delta operator has not changed under the action of this transformation.

The rotational transformation, denoted textually [11] by the unitary operator \hat{R} , is a member of the Galilean group of transformations. As a consequence, it is realizable that the Weyl transform $A^W(pq)$ should also

exhibit rotational invariance. However, 3-dimensions are required to fully appreciate rotational symmetry and thus p and q must be replaced by their respective vector quantities \mathbf{p} and \mathbf{q} . But for simplicity we are restricting our examination of pseudo phase space to only 1-dimension. We shall, therefore, accept rotational invariance on face value. (Kruger and Poffyn, [14], consider in some detail all elements of the Galilean group of transformations, which also includes rotation. However, their discussion is very general but the gist of the argument is self explanatory).

The parity transformation of $A^W(pq)$ can be found by using equation (1.3.16) on the transformed operator $\hat{A}' = \hat{\Pi}\hat{A}\hat{\Pi}^+$, namely

$$\begin{aligned}
 A'^W(pq) &= \int \exp\left\{\frac{i}{\hbar} p v\right\} \langle q - \frac{1}{2} v | \hat{A}' | q + \frac{1}{2} v \rangle dv \\
 &= \int \exp\left\{\frac{i}{\hbar} p v\right\} \langle q - \frac{1}{2} v | \hat{\Pi}\hat{A}\hat{\Pi}^+ | q + \frac{1}{2} v \rangle dv \\
 &= \int \exp\left\{\frac{i}{\hbar} p v\right\} \langle q - \frac{1}{2} v | r \rangle \langle -r | \hat{A} | -s \rangle \langle s | q + \frac{1}{2} v \rangle dv dr ds \\
 &= A^W(-p, -q)
 \end{aligned} \tag{1.8.6}$$

Hence, parity inverts both pseudo phase space variables.

We have not explicitly introduced the time variable into the definition of the Weyl transform but we can still obtain the time reversal symmetry. To accomplish this we shall need a special type of operator whose action upon a wave-function is to transform it into its complex conjugate. Such an operator of conjugation is called an anti-linear operator denoted by \hat{T} , [11], which has the property that

$$\hat{T}(a_1|\psi_1\rangle + a_2|\varphi_2\rangle) = a_1^*(\hat{T}|\psi_1\rangle) + a_2^*(\hat{T}|\varphi_2\rangle) \quad (1.8.7)$$

where a_1 and a_2 are arbitrary complex numbers.

If, in addition, \hat{T} satisfies the condition

$$\hat{T}^\dagger \hat{T} = \hat{T} \hat{T}^\dagger = 1 \quad (1.8.8)$$

then \hat{T} is an anti-unitary operator.

Using equation (1.8.7) we find for the scalar product that

$$\langle \psi | (\hat{T}|\varphi\rangle) = \left[\langle \psi | \hat{T} | \varphi \rangle \right]^* \quad (1.8.9)$$

With the exception of equations (1.8.7) and (1.8.9) anti-unitary operators satisfy all the properties of unitary operators. Therefore, we have specifically an anti-unitary transformation of an arbitrary linear operator \hat{A} given by

$$\hat{A}' = \hat{T} \hat{A} \hat{T}^\dagger \quad (1.8.10)$$

Because time reversal as the effect of conjugating the wave-function, [11], the anti-unitary operator \hat{T} is often referred to as the time reversal operator. It is by using \hat{T} that we shall obtain the time reversal of the Weyl transform.

The Weyl transform of the linear operator \hat{A} is, from equation (1.3.16),

$$A^w(pq) = \int \exp\left\{\frac{i}{\hbar} p v\right\} \langle q - \frac{1}{2} v | \hat{A} | q + \frac{1}{2} v \rangle dv$$

$$\begin{aligned}
&= \int \exp\left\{\frac{i}{\hbar} p v\right\} \langle q - \frac{1}{2} v | \hat{T}^+ \hat{A} \hat{T} | q + \frac{1}{2} v \rangle dv \\
&= \int \exp\left\{\frac{i}{\hbar} p v\right\} \left[\langle q - \frac{1}{2} v | \hat{T}^+ \right] \hat{A}' \left[\hat{T} | q + \frac{1}{2} v \rangle \right]^* dv \\
&= \left[\int \exp\left\{\frac{i}{\hbar} (-p) v\right\} \langle q - \frac{1}{2} v | \hat{T}^+ \right] \hat{A}' \left[\hat{T} | q + \frac{1}{2} v \rangle \right]^* dv \\
&= \left[A'^W(p', q') \right]^* \tag{1.8.11}
\end{aligned}$$

where we have used equations (1.8.9) and (1.8.10). Also, we have taken $\langle q - v/2 | \hat{T}^+$ and $\hat{T} | q + v/2 \rangle$ as the transformed vectors $\langle q' - v/2 |$ and $| q' + v/2 \rangle$ and $p' = -p$. So that, finally we can write

$$A^W(pq) = \left[A'^W(-pq) \right]^* \tag{1.8.12}$$

Time reversal, as we would expect, inverts the momentum variable and leaves the position variable unchanged. However, note that the rhs of equation (1.8.12) is the complex conjugate of $A'^W(-pq)$. Thus reminding us that Weyl transforms are not in general real functions in pseudo phase space. If the operator \hat{A} represents an observable quantity, ie \hat{A} is Hermitian, then the Weyl transform will be real and

$$A^W(pq) = A'^W(-pq) \tag{1.8.13}$$

As an example we shall find the time reversal of the commutation rule

$$[\hat{p}, \hat{q}]_t = -i\hbar \quad (1.8.14)$$

Replacing t by $-t$ and using equation (1.8.10) in (1.8.14) gives

$$\begin{aligned} [\hat{p}, \hat{q}]_{-t} &= \hat{T}(-i\hbar)\hat{T}^+ \\ &= i\hbar \end{aligned} \quad (1.8.15)$$

Applying equation (1.8.12) to the last two examples of Section (1.4) yields

$$(\hat{p}\hat{q})_{-t} \begin{matrix} \Rightarrow \\ \Leftarrow \end{matrix} -pq + \frac{i\hbar}{2} \quad (1.8.16a)$$

$$(\hat{q}\hat{p})_{-t} \begin{matrix} \Rightarrow \\ \Leftarrow \end{matrix} -qp - \frac{i\hbar}{2} \quad (1.8.16b)$$

Subtracting equation (1.8.16b) from (1.8.16a) gives at once

$$[\hat{p}, \hat{q}]_{-t} \begin{matrix} \Rightarrow \\ \Leftarrow \end{matrix} i\hbar \quad (1.8.17)$$

1.9 SYMPLECTIC FORM OF THE WEYL CORRESPONDENCE

We have, so far, restricted the discussion to one dimensional pseudo phase space. In this Section we shall generalise Weyls' rule by using what as become known as symplectic notation, [15,16]. Symplectic notation is the interweaving of the n generalised position and momentum co-ordinates such that

$$\begin{aligned}x^\alpha &= q^\alpha \\x^{\alpha+n} &= p^\alpha\end{aligned}\tag{1.9.1}$$

where α ranges from $1, 2, \dots, n$.

Using equation (1.9.1) we are able to write Hamiltons equations as a single expression, namely

$$\dot{x}^\alpha = \epsilon^{\alpha\beta} \frac{\partial H}{\partial x^\beta}\tag{1.9.2}$$

where $\alpha, \beta = 1, 2, \dots, 2n$ and $\epsilon^{\alpha\beta}$ can be written in terms of the Kronecker delta, as

$$\epsilon^{\alpha\beta} = \delta^{\beta, \alpha+n} - \delta^{\beta, \alpha-n}\tag{1.9.3}$$

or, alternatively, as the elements of the $2n \times 2n$ matrix

$$\epsilon = \begin{Bmatrix} 0 & I \\ -I & 0 \end{Bmatrix}\tag{1.9.4}$$

where 0 and I are the nxn zero and unit matrices. Its is straightforward to show that ϵ is anti-symmetric, orthogonal and has a unit determinant.

Symplectic notation has found an application in pseudo phase space as a compact and, somewhat, mathematically elegant method for obtaining Weyl transforms of multinomial functions, [17]. This shall now be demonstrated. In symplectic notation equations (1.2.3), (1.2.4) and (1.3.15) can be re-written as

$$\hat{A} = \frac{1}{h} \int A^W(x^\alpha) \hat{\Delta}_x^\alpha dx^\alpha \quad (1.9.5)$$

$$\hat{\Delta}_x^\alpha = \frac{1}{h} \int \exp\left\{\frac{i}{h}(x^\alpha - \hat{x}^\alpha)u^\alpha\right\} du^\alpha \quad (1.9.6)$$

and

$$A^W(x^\alpha) = \text{Tr}[\hat{A} \hat{\Delta}_x^\alpha] \quad (1.9.7)$$

There is not a great deal that can be learnt from the symplectic generalisations of equations (1.2.3), (1.2.4) and (1.3.15). However, symplectic form is more suited for finding Weyl transforms of general products. To see this we shall need an extension of the BCH Theorem, equation (1.3.1), this is given by, (see appendix of reference [17]),

$$\exp\{\hat{A}_1 + \dots \hat{A}_n\} = \exp\{\hat{A}_1\} \dots \exp\{\hat{A}_n\} \exp\left\{-\frac{1}{2} \sum_{j < k} [\hat{A}_j, \hat{A}_k]\right\} \quad (1.9.8)$$

where

$$[[\hat{A}_i, \hat{A}_j], \hat{A}_k] = 0 \quad (1.9.9)$$

with i, j and $k = 1, 2, \dots, n$.

From equation (1.9.5), we have

$$\hat{A}_1 \dots \hat{A}_n = \frac{1}{h^n} \int A_1^w(x^\alpha) \dots A_n^w(x^\alpha) \hat{\Delta}_{x_1^\alpha} \dots \hat{\Delta}_{x_n^\alpha} dx_1^\alpha \dots dx_n^\alpha \quad (1.9.10)$$

where the order of the $\hat{\Delta}_{x^\alpha}$ is important.

By iteration and using equation (1.9.8) we have

$$\hat{\Delta}_{x_1^\alpha} \dots \hat{\Delta}_{x_n^\alpha} = h^{n-1} \exp \left\{ \frac{i\hbar}{2} \sum_{j < k} \epsilon^{\alpha\beta} \frac{\partial^2}{\partial x_j^\alpha \partial x_k^\beta} \right\} \prod_{j < k} \delta(x_j^\alpha - x_k^\alpha) \hat{\Delta}_{x_1^\alpha} \quad (1.9.11)$$

Substituting equation (1.9.11) into (1.9.10) and carrying out a iterative partial integration yields

$$\hat{A}_1 \dots \hat{A}_n = \frac{1}{h} \int \left[\exp \left\{ \frac{i\hbar}{2} \sum_{j < k} \epsilon^{\alpha\beta} \frac{\partial^2}{\partial x_j^\alpha \partial x_k^\beta} \right\} A^w(x^\alpha) \dots A^w(x^\alpha) \right] \hat{\Delta}_{x_1^\alpha} dx_1^\alpha \quad (1.9.12)$$

Comparing equation (1.9.12) with (1.9.5) finally gives

$$[\hat{A}_1 \dots \hat{A}_n]_{x^\alpha}^w = \exp \left\{ \frac{i\hbar}{2} \sum_{j < k} \epsilon^{\alpha\beta} \frac{\partial^2}{\partial x_j^\alpha \partial x_k^\beta} \right\} A_1^w(x^\alpha) \dots A_n^w(x^\alpha) \quad (1.9.13)$$

Equation (1.9.13) displays the mathematical elegance of symplectic notation for generating Weyl transforms of products of operators.

Reversing the order of the operators in equation (1.9.13) negates the argument of the exponential, so that

$$[\hat{A}_n \dots \hat{A}_1]_{x^\alpha}^w = \exp \left\{ - \frac{i\hbar}{2} \sum_{j < k} \epsilon^{\alpha\beta} \frac{\partial^2}{\partial x_j^\alpha \partial x_k^\beta} \right\} A_1^w(x^\alpha) \dots A_n^w(x^\alpha) \quad (1.9.14)$$

Setting $n=2$ in equation (1.9.13) and using equation (1.9.4) gives

$$[\hat{A}_1 \hat{A}_2]_{x^\alpha}^w = \exp \left\{ \frac{i\hbar}{2} \left[\frac{\partial}{\partial x_1^\alpha} \frac{\partial}{\partial x_2^\alpha} - \frac{\partial}{\partial x_2^\alpha} \frac{\partial}{\partial x_1^\alpha} \right] \right\} A_1^w(x^\alpha) A_2^w(x^\alpha) \quad (1.9.15)$$

Allowing α to extend only over one dimensional pseudo phase space we can identify at once equation (1.9.15) with (1.3.19).

As a consequence Groenewolds' rule, equation (1.3.20), assumes the elegant re-statement

$$[\hat{A}_1, \hat{A}_2]_{x^\alpha}^w = A_1^w \left[x^\alpha + \frac{i\hbar}{2} \epsilon^{\alpha\beta} \frac{\partial^2}{\partial x^\alpha} \right] A_2^w(x^\alpha)$$

$$= A_2^w \left[x^\alpha - \frac{i\hbar}{2} \epsilon^{\alpha\beta} \frac{\partial^2}{\partial x^\alpha} \right] A_1^w(x^\alpha) \quad (1.9.16)$$

In summary, the symplectic form of Weyls' correspondence rule is only advantageous for finding Weyl transforms of products of operators. However, it has its limitations as well. For instance, consider the lhs of equation (1.9.13). This can be written, using equation (1.9.7), as

$$[\hat{A}_1 \dots \hat{A}_n]_{x^\alpha}^w = \text{Tr} [\hat{\Delta}_{x^\alpha} (\hat{A}_1 \dots \hat{A}_n)] \quad (1.9.17)$$

Let the \hat{A}_n be replaced by delta operators ranging from 1 to $n-1$. Then the rhs of equation (1.9.17) becomes a trace of n delta operators, namely

$$\text{Tr} [\hat{\Delta}_{x^\alpha} \hat{\Delta}_{x_1^\alpha} \dots \hat{\Delta}_{x_{n-1}^\alpha}] \quad (1.9.18)$$

Equation (1.9.18) assumes two different forms depending on whether n is even or odd, [1]. To prove this by using the rhs of equation (1.9.13) results in tedious algebraic manipulations of δ -functions.

CHAPTER TWO

THE WIGNER FUNCTION

2.1 INTRODUCTION

In 1932, Wigner [18], wrote down a probability type function of both position and momentum variables[#]. Wigners' quasi-probability function enabled him to calculate the quantum corrections to classical results for a statistical system in thermal equilibrium. The corrections were expressed as a power series in \hbar . This function is called the Wigner distribution function and shall be denoted by $P^W(pq)$. As we shall see, the Wigner function is essentially the Weyl transform of the von Neumann density matrix $\hat{\rho}$. Its use is analogous to that of the classical probability density function. For instance, as Wigner pointed out, if we take an operator \hat{A} that can be written as the sum

$$\hat{A} = f(\hat{p}) + g(\hat{q})$$

where \hat{p} and \hat{q} are the usual operators corresponding to linear momentum and position, then the expectation value of \hat{A} , namely $\text{Tr}(\hat{\rho}\hat{A})$, can be calculated in the normal (ie classical) way as

$$\langle \hat{A} \rangle = \int [f(p) + g(q)] P^W(pq) dp dq$$

This portrayal is classical in appearance but $P^W(pq)$ is a completely quantum object and the result of using it to calculate expectation values is fully quantum mechanical.

[#] In his paper, Wigner dismisses in a handwaving gesture how and why the function was first obtained. However, as he does remark, it is the simplest from a wide class of such functions.

Moyal, [19], extended this to include arbitrary operators which can be expressed as a function $f(\hat{p}, \hat{q})$, the proviso being that one must first apply Weyl's rule of association to $f(\hat{p}, \hat{q})$. This is given explicitly in Section 2.3. In his paper, Moyal set down the general mathematical structure outlining the reformulation of quantum mechanics in pseudo phase space. He pointed out that for this formulation to be practicable it is essential that one first takes the Weyl transforms of the operators. Furthermore, he showed that the Wigner function arises naturally from the Fourier inverse of the statistical characteristic function.

As a fully quantum object the Wigner function does, of course, have its non-classical aspects. It cannot for example be interpreted as a true joint probability function in both position and momentum. This is due to its being able to take negative values for some values of p and q . (The Wigner function corresponding to all pure states can take negative values in some regions of pseudo phase space, with the exception of Gaussian states for which the Wigner function is always non-negative, [21,22]. Many mixed states do, however, possess non-negative Wigner functions). Because of this property, the Wigner function is often described as a quasi-probability function.

There are alternatives to the Wigner function. Some of these functions, depending on the correspondence rule used to obtain them, can even become imaginary for some values of p and q . We shall not concern ourselves with these more complicated distribution functions.

One should not discard the pseudo phase space formulation, for its formal classical appearance, when calculating moments, makes it very appealing. In fact, the Wigner function has found applications in just about all branches of mathematical physics.

This chapter will be dedicated solely to the Wigner function. In Section 2.2 we shall show that the Wigner function is proportional to the

Weyl transform of the von Neumann, [20], density matrix $\hat{\rho}$ where the constant of proportionality is just the reciprocal of Planck's constant, h . In addition, we see how the characteristic function of Moyal is embedded in our delta operator, $\hat{\Delta}_{pq}$. This then enables us to display the relationship between the statistical characteristic function and the Wigner function. The resemblance of the formalism here to that of classical statistical mechanics forms the subject of Section 2.3. In Section 2.4 we list some of the important properties of the Wigner function. The "transport" equation of motion for the Wigner function is derived in Section 2.5. It is the pseudo phase space equivalent to the equation of motion for von Neumanns' density matrix, $\hat{\rho}$; taking the Weyl transform of that equation yields the equation of motion for $P^W(pq)$. Finally, in Section 2.6 we discuss the Wigner function for thermal equilibrium by first finding the Weyl transform of $\exp\{-\beta\hat{H}\}$. As an example, the Wigner function for the thermal oscillator is obtained. We conclude the section, and chapter, with an alternative method for finding the Weyl transform of $\exp\{-\beta\hat{H}\}$.

2.2 WEYL TRANSFORM OF THE DENSITY MATRIX

The state of a system is completely described by the von Neumann density matrix $\hat{\rho}$. In terms of the normalized eigenfunctions $|\psi_n\rangle$ we have

$$\hat{\rho} = \sum_n \omega_n |\psi_n\rangle\langle\psi_n| \quad (2.2.1))$$

where ω_n is the statistical weight subject to the two restrictions

$$\omega_n > 0 \quad \text{and} \quad \sum_n \omega_n = 1$$

It follows from the above definition that

$$\text{Tr}[\hat{\rho}] = 1 \quad \text{and} \quad \text{Tr}[\hat{\rho}^2] \leq 1 \quad (2.2.2)$$

The equality in the second of equations (2.2.2) holds for pure states only, for which $\hat{\rho}^2 = \hat{\rho}$ (the property of idempotency), where all but one ω are zero, this having the value of unity. In fact the idempotency of $\hat{\rho}$ is a necessary and sufficient central condition for $\hat{\rho}$ to describe a pure state.

The Wigner function can be defined as the Weyl transform of $\hat{\rho}/h$. If we replace the operator \hat{A} by $\hat{\rho}$, of equation (2.2.1), in equation (1.3.16) and divide by h we recover at once the Wigner function, as

$$p^w(pq) = \frac{1}{h} \left[\hat{\rho} \right]_{pq}^w$$

$$= \frac{1}{h} \text{Tr}[\hat{\rho} \hat{\Delta}_{pq}]$$

$$= \frac{1}{h} \sum_n \omega_n \int \exp\left\{\frac{i}{h} p v\right\} \psi_n^*(q + \frac{1}{2} v) \psi_n(q - \frac{1}{2} v) dv \quad (2.2.3)$$

For simplicity we shall consider only pure states unless stated otherwise, bearing in mind that all results can be easily generalised to include mixed states.

Thus, for pure states, equation (2.2.3) becomes

$$P^W(pq) = \frac{1}{h} \int \exp\left\{\frac{i}{h} p v\right\} \psi^*(q + \frac{1}{2} v) \psi(q - \frac{1}{2} v) dv \quad (2.2.4)$$

We know from ordinary quantum mechanics, [11], that the expectation value of an operator \hat{A} can be written as

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle \quad (2.2.5)$$

Substituting for \hat{A} of equation (1.2.3) into rhs of equation (2.2.5) we have

$$\langle \hat{A} \rangle = \frac{1}{h} \int A^W(pq) \langle \psi | \hat{\Delta}_{pq} | \psi \rangle dp dq \quad (2.2.6)$$

Using equation (1.2.4) we have

$$\frac{1}{h} \langle \psi | \hat{\Delta}_{pq} | \psi \rangle = \frac{1}{h^2} \int \exp\left\{\frac{i}{h}(p v + q u)\right\} C^F(u, v) du dv \quad (2.2.7)$$

where

$$C^F(u,v) = \langle \psi | \exp \left\{ -\frac{i}{\hbar} (\hat{p}v + \hat{q}u) \right\} | \psi \rangle \quad (2.2.8)$$

is the characteristic function.

In addition, comparing equation (2.2.8) with (1.7.18) the characteristic function is just the expectation value of the pseudo phase space displacement operator, namely

$$C^F(u,v) = \langle \psi | \hat{D}_{uv} | \psi \rangle \quad (2.2.9)$$

The lhs of equation (2.2.7) is just another way of writing $P^W(pq)$. To see this we make use of an extension to the BCH Theorem [10], namely

$$\exp\{\hat{A} + \hat{B}\} = \exp\left\{\frac{1}{2} \hat{B}\right\} \exp\{\hat{A}\} \exp\left\{\frac{1}{2} \hat{B}\right\} \quad (2.2.10)$$

Using equation (1.2.4) and applying equation (2.2.10) to the lhs of equation (2.2.7) we find, after a little algebra, that

$$P^W(pq) = \frac{1}{\hbar} \langle \psi | \hat{\Delta}_{pq} | \psi \rangle \quad (2.2.11)$$

Hence, equation (2.2.7) becomes

$$P^W(pq) = \frac{1}{\hbar^2} \int \exp\left\{\frac{i}{\hbar} (pv + qu)\right\} C^F(u,v) du dv \quad (2.2.12)$$

So that the Wigner function is the Fourier transform of the (quantum) statistical characteristic function.

Another way of arriving at equation (2.2.11) is as follows:

$$\begin{aligned}
 \frac{1}{\hbar} \langle \psi | \hat{\Delta}_{pq} | \psi \rangle &= \frac{1}{\hbar} \text{Tr} \left[| \psi \rangle \langle \psi | \hat{\Delta}_{pq} \right] \\
 &= \frac{1}{\hbar} \left[| \psi \rangle \langle \psi | \right]_{pq}^w \\
 &= \frac{1}{\hbar} \left[\hat{\rho} \right]_{pq}^w \\
 &= P^w(pq)
 \end{aligned} \tag{2.2.13}$$

As an observation, the Wigner function follows directly from the matrix elements of $\hat{\rho}$ and vice versa. Inverting equation (2.2.4) gives

$$\langle q - \frac{1}{2} v | \hat{\rho} | q + \frac{1}{2} v \rangle = \int \exp \left\{ -\frac{i}{\hbar} p v \right\} P^w(pq) dp \tag{2.2.14}$$

Thus one may see that the Wigner function contains the same amount of information about the system as does $\hat{\rho}$.

2.3 CLASSICAL FEATURES OF THE WIGNER FUNCTION

In Section 2.4, property 10, we shall find that, the Wigner function is not, in general, everywhere non-negative. For this reason it cannot be

considered a true probability distribution function in the classical sense. However, it does in many ways closely resemble a probability distribution function. It will shortly be shown in detail that the Wigner function even possesses some of the properties akin to a classical distribution function (cf Section 2.4).

For now we shall demonstrate, with the help of the Weyl correspondence, the formal classical resemblance of the Wigner function. Consider the quantum mechanical average of the operator \hat{A}

$$\langle A \rangle = \text{Tr}[\hat{A}\hat{\rho}] \quad (2.3.1)$$

What we can do, by using definition (1.3.22), is to transform equation (2.3.1) into a pseudo phase space integral as

$$\langle \hat{A} \rangle = \frac{1}{h} \int A^W(pq) (\hat{\rho})_{pq}^W dp dq \quad (2.3.2)$$

$$= \int A^W(pq) P^W(pq) dp dq \quad (2.3.3)$$

Equation (2.3.3) is a result of Moyal, [19], based on Wigners' original definition and applies for any state $\hat{\rho}$, not just pure states. Recall, [15], that the classical average with respect to the classical phase space function $A(pq)$, is

$$\langle A(pq) \rangle = \int A(pq) P^{cl}(pq) dp dq \quad (2.3.4)$$

where $P^{cl}(pq)$ is the classical probability distribution function in phase space.

Thus, upon comparison of equations (2.3.3) and (2.3.4) we observe the distinctive formal similarity. It must be remembered, of course, that equation (2.3.3) is completely quantum. It is only in the classical limit, where $\hbar \rightarrow 0$ and pseudo phase space goes over to classical phase space, that equation (2.3.3) becomes identical to equation (2.3.4).

2.4 PROPERTIES OF THE WIGNER FUNCTION

The Wigner function possesses many intrinsic properties. Through these properties we are able to gain an insight into the fundamental significance of this function. That is, to help understand why it can be used as a probability-type function and to suggest features of its geometrical structure. We shall now expound the more important of these properties and present them in a numerical list.

1) The Wigner function is real.

We know that the Wigner function is proportional to the Weyl transform of the density matrix $\hat{\rho}$ and also that $\hat{\rho}$ is Hermitian. Therefore, by the properties of the Weyl transform we conclude that the Wigner function is real.

2) The Wigner function is normalized to unity.

Integration of equation (2.2.4) over the pseudo phase space variables p, q yields at once

$$\int P^W(pq) dp dq = 1 \quad (2.4.1)$$

This corresponds to the fact that $\text{Tr}[\hat{\rho}] = 1$, for any state $\hat{\rho}$.

3) The Wigner function produces the customary marginal probabilities.

Integration of equation (2.2.4) over p gives

$$\int P^W(pq) dp = |\psi(q)|^2 \quad (2.4.2)$$

and over q gives

$$\int P^W(pq) dq = |\varphi(p)|^2 \quad (2.4.3)$$

where $\varphi(p)$ is the momentum space wave function and is related to $\psi(q)$ by the Fourier integral

$$\psi(q) = \frac{1}{\sqrt{h}} \int \exp\left\{\frac{i}{h} pq\right\} \varphi(p) dp \quad (2.4.4)$$

4) The Wigner function is bounded, [1] [24].

The Wigner function for a pure state can be written, by using equation (2.2.11), as

$$P^W(pq) = \frac{1}{h} \langle \psi | \hat{\Delta}_{pq} | \psi \rangle$$

$$= \frac{2}{h} \langle \psi | \hat{\Pi}_{pq} | \psi \rangle$$

$$= \frac{2}{h} \langle \psi | \psi^R \rangle \quad (2.4.5)$$

where in the second step we have used equation (1.6.9).

Applying Schwarz's inequality

$$|\langle \varphi | \psi \rangle|^2 \leq \langle \varphi | \varphi \rangle \langle \psi | \psi \rangle \quad (2.4.6)$$

to equation (2.4.5), gives

$$\begin{aligned} |P^W(pq)| &= \frac{2}{h} |\langle \psi | \psi^R \rangle| \\ &\leq \frac{2}{h} \left[\langle \psi | \psi \rangle \langle \psi^R | \psi^R \rangle \right]^{\frac{1}{2}} \\ &= \frac{2}{h} \end{aligned} \quad (2.4.7)$$

where we have used equation (1.6.7). Hence, $P^W(pq)$ for pure states must lie between $+2/h$ and $-2/h$.

Royer, [12], has shown that the upper (lower) bound for $P^W(pq)$, for pure states, is attained when ψ is symmetric (anti-symmetric). Other values within the bounded interval are obtained for ψ having both symmetric and anti-symmetric parts.

5) The Galilean invariance of the Wigner function.

Equation (2.2.4) represents the Wigner function for pure states. It has been defined in the non-relativistic limit and is applicable only to spinless particles. Therefore, a natural property should be that the Wigner function is Galilean invariant. These invariance properties follow directly from Section 1.8, since the Wigner function is just a special case of the

Weyl transform. Hence, we conclude that the Wigner function is invariant under the Galilean group of transformations.

6) The Wigner function is parity invariant.

This follows immediately from equation (1.8.6), which gives the co-ordinate inversion $P^W(-p, -q)$.

7) The Wigner function is invariant under time reversal.

This follows directly from equation (1.8.13) and property 1, to get $P^W(-p, q)$.

8) The Wigner function does not satisfy an "idempotency" condition.

For pure states we know that $\hat{\rho} = \hat{\rho}^2$. This characteristic is not mirrored in the Wigner-Weyl picture. This can be seen by taking the Weyl transform of $\hat{\rho} = \hat{\rho}^2$. Thus, using equation (1.3.19) we have

$$P^W(pq) = h P^W(pq) \exp \left\{ \frac{i\hbar}{2} \left[\frac{\overleftarrow{\partial}}{\partial q} \frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p} \frac{\overrightarrow{\partial}}{\partial q} \right] \right\} P^W(pq)$$

$$\neq h [P^W(pq)]^2 \quad (2.4.8)$$

The last two properties to be discussed will indirectly suggest the form of the Wigner function.

9) The Wigner function is not a δ -function.

Since we are only considering pure states then

$$\hat{\rho}^2 = \hat{\rho} \quad (2.4.9)$$

Taking the trace of both sides of equation (2.4.9) gives

$$\text{Tr}[\hat{\rho}^2] = 1 \quad (2.4.10)$$

By equation (1.3.22) the lhs of equation (2.4.10) becomes

$$h \int [P^W(pq)]^2 dp dq = 1 \quad (2.4.11)$$

Equation (2.4.11) shows that the Wigner function is not too sharply defined and implicitly suggests that $P^W(pq)$ cannot be a δ -function.

Another way to see this is by first supposing that the Wigner function is a δ -function, ie $P^W(pq) = \delta(p - p')\delta(q - q')$. We shall use the Heisenburg uncertainty principle to obtain a contradiction. Substituting the assumed Wigner function into equation (2.3.3) gives

$$\langle \hat{A} \rangle = A^W(p'q') \quad (2.4.12)$$

Equation (2.4.12) says that the expectation value of any quantum operator \hat{A} is just its Weyl transform. (This in itself appears to be resting on shaky ground, particularly when \hat{A} is a function of a product of \hat{p} and \hat{q} . Because we demand that $\langle \hat{A} \rangle$ must be in all cases a real quantity).

If the Wigner function were a δ -function, Weyl transforms of the first and second moments of \hat{p} and \hat{q} would be

$$\langle \hat{p} \rangle \xrightarrow{\leftarrow} p \quad (2.4.13a)$$

$$\langle \hat{p}^2 \rangle \xrightarrow{\leftarrow} p^2 \quad (2.4.13b)$$

$$\langle \hat{q} \rangle \begin{matrix} \rightarrow \\ \leftarrow \end{matrix} q \quad (2.4.13c)$$

$$\langle \hat{q}^2 \rangle \begin{matrix} \rightarrow \\ \leftarrow \end{matrix} q^2 \quad (2.4.13d)$$

which gives us at once the uncertainty relation $\Delta p \Delta q = 0$. So we have a contradiction and conclude that the Wigner function cannot be a δ -function. In addition, we can see that a δ -function form for $P^W(pq)$ would not meet the criterion of equation (2.4.7), which all Wigner functions must satisfy. (However, in the classical limit, $\hbar \rightarrow 0$, a δ -function form for $P^{cl}(pq)$ can be an acceptable distribution).

10) The Wigner function, for pure states, can take negative values in some regions of pseudo phase space.

In previous Sections we have mentioned that the Wigner function may assume negative values for some p and q , [25,26]. The first (but not the simplest) proof rigorously to show that Wigner functions for all pure states must be negative for some regions of pseudo phase space was given by Wigner, [26]. An alternative, and simpler, way to see this is as follows:

If $|\psi\rangle$ and $|\varphi\rangle$ are two arbitrary orthogonal state vectors, then we have by definition $\langle \varphi | \psi \rangle = 0$ and consequently $|\langle \varphi | \psi \rangle|^2 = 0$. But

$$\begin{aligned} |\langle \varphi | \psi \rangle|^2 &= \text{Tr} [|\varphi\rangle \langle \varphi| \cdot |\psi\rangle \langle \psi|] \\ &= \text{Tr} [\hat{\rho}_\varphi \hat{\rho}_\psi] \\ &= h \int P_\varphi^W(pq) P_\psi^W(pq) dp dq \end{aligned} \quad (2.4.14)$$

where we have used equation (1.3.22) to obtain the last expression.

Since equation (2.4.14) must be equated to zero the integral must vanish. That is, at least one of the $P_{\phi}^W(pq)$ or $P_{\psi}^W(pq)$ must be negative within the interval of integration. Thus, we conclude that for pure states the Wigner function will generally be negative on some regions of pseudo phase space.

Indeed, Gaussian states are the only pure states with non-negative Wigner functions, [21], but many mixed states have corresponding Wigner functions that are non-negative for all p and q . (cf Section 2.6, where we obtain a Wigner function for a mixed state which exhibits this property). The criteria for determining which mixed states will produce non-negative Wigner functions remains, at present, an unresolved question.

2.5 TIME DEVELOPMENT OF THE WIGNER FUNCTION

In general, $P^W(pq)$, is time dependent and consequently its time evolution will be governed by an equation of motion. This equation of motion can be found by differentiating equation (2.2.4) with respect to time, t , and using Schroedingers' equation

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x,t)\psi(x,t) \quad (2.5.1a)$$

and its complex conjugate

$$-i\hbar \frac{\partial \psi^*(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi^*(x,t)}{\partial x^2} + V(x,t)\psi^*(x,t) \quad (2.5.1b)$$

A more direct route (following, for instance, reference [1]) is to use von Neumanns', [20], equation of motion for $\hat{\rho}$, namely

$$\frac{\partial \hat{\rho}}{\partial t} = - \frac{i}{\hbar} [\hat{H}, \hat{\rho}] \quad (2.5.2)$$

where

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q}, t) \quad (2.5.3)$$

is the Hamiltonian operator.

We can take the Weyl transform of both sides of equation (2.5.2) using our earlier definitions (especially (1.3.19)) to get for the equation of motion for $P^W(pq)$

$$\frac{\partial P^W(pqt)}{\partial t} = \frac{2}{\hbar} H^W(pqt) \sin \left\{ \frac{\hbar}{2} \left[\frac{\overleftarrow{\partial}}{\partial q} \frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p} \frac{\overrightarrow{\partial}}{\partial q} \right] \right\} P^W(pqt) \quad (2.5.4)$$

which is the quantum analogue of Liouville's equation. It is worth emphasizing that equation (2.5.4) holds for general mixed states.

We are considering Hamiltonians with Weyl transform given by

$$H^W(pqt) = \frac{p^2}{2m} + V(q, t) = H(pqt) \quad (2.5.5)$$

In this case equation (2.5.4) reduces to

$$\frac{\partial P^W(pqt)}{\partial t} = -\frac{p}{m} \frac{\partial P^W(pqt)}{\partial q} + \frac{2}{\hbar} V(q,t) \sin \left[\frac{\hbar}{2} \frac{\overleftarrow{\partial}}{\partial q} \frac{\overrightarrow{\partial}}{\partial p} \right] P^W(pqt) \quad (2.5.6)$$

We will note some interesting consequences of equation (2.5.6). For instance, considering potentials that are up to and including quadratic terms in q (the harmonic oscillator) we find that equation (2.5.6) specialises to

$$\frac{\partial P^W(pqt)}{\partial t} = \frac{\partial H(pqt)}{\partial q} \frac{\partial P^W(pqt)}{\partial p} - \frac{\partial H(pqt)}{\partial p} \frac{\partial P^W(pqt)}{\partial q} \quad (2.5.7)$$

which is independent of \hbar but still fully quantum. Equation (2.5.7) is the 'classical' Liouville equation.

One may be wondering about the apparent disappearance of quantum mechanics for these quadratic potentials. Even in the special case of equation (2.5.7) there is quantum mechanical content; it is contained within the the initial structure of $P^W(pq)$. Again we see similarities with classical phase space methods manifesting themselves. However, as the order of the potential increases beyond quadratic, \hbar enters into the equation and obtaining analytical solutions is often difficult.

Another interesting point to consider is the transition to the classical regime. Taking \hbar to zero in equation (2.5.4) or (2.5.6) gives, devoid of any singularities, the well known classical Liouville equation, [15],

$$\frac{\partial P^{cl}(pqt)}{\partial t} = \frac{\partial H(pqt)}{\partial q} \frac{\partial P^{cl}(pqt)}{\partial p} - \frac{\partial H(pqt)}{\partial p} \frac{\partial P^{cl}(pqt)}{\partial q} \quad (2.5.8)$$

Equation (2.5.8) displays the ease in which the prescription for the classical limit can be applied.

2.6 WIGNER FUNCTION FOR THERMAL EQUILIBRIUM

In quantum mechanics, a particular member of the ensemble in thermal equilibrium occupies a particular energy level with a probability given by the density matrix $\hat{\rho}$. This is given by the well known distribution

$$\hat{\rho} = \frac{\exp\{-\beta\hat{H}\}}{\text{Tr}[\exp\{-\beta\hat{H}\}]} \quad (2.6.1)$$

where \hat{H} is the (time independent) Hamiltonian operator, $\beta=1/kT$ with k the Boltzmann constant and T the absolute temperature, and the normalization factor $\text{Tr}[\exp\{-\beta\hat{H}\}]$ is called the partition function and usually denoted by Z .

It follows at once, from equation (2.6.1), that $\text{Tr}[\hat{\rho}] = 1$. The expectation values of an operator \hat{A} for an ensemble distributed in accordance to equation (2.6.1) is, by equation (2.3.1)

$$\langle \hat{A} \rangle = \frac{\text{Tr}[\hat{A} \exp\{-\beta\hat{H}\}]}{\text{Tr}[\exp\{-\beta\hat{H}\}]} \quad (2.6.2)$$

With the aid of equations (1.3.21) and (1.3.22) we can re-express the expectation as

$$\langle \hat{A} \rangle = \frac{\int A^w(pq) [\exp\{-\beta \hat{H}\}]_{pq}^w dp dq}{\int [\exp\{-\beta \hat{H}\}]_{pq}^w dp dq} \quad (2.6.3)$$

At first sight the task of determining the Weyl transform of $\exp\{-\beta \hat{H}\}$ appears to be a daunting one since an expansion of the exponential generates factors of increasing powers of \hat{H} , where each such term it contains must be Weyl transformed. Another way to proceed is to differentiate equation (2.6.1) with respect to β to get the Bloch equation, [27],

$$\frac{\partial \hat{\rho}}{\partial \beta} = - \hat{H} \hat{\rho} \quad (2.6.4)$$

In this case of thermal equilibrium, \hat{H} and $\hat{\rho}$ commute and we can employ a useful trick and write the rhs of equation (2.6.4) as an anti-commutator, thus

$$\frac{\partial \hat{\rho}}{\partial \beta} = - \frac{1}{2} \{\hat{H}, \hat{\rho}\} \quad (2.6.5)$$

where $\{\hat{H}, \hat{\rho}\} \equiv \hat{H} \hat{\rho} + \hat{\rho} \hat{H}$.

We can take the Weyl transform of equation (2.6.5) by noting that the Weyl transform of the rhs is just minus the real part of equation (1.3.19),

to get

$$\frac{\partial [\exp\{-\beta\hat{H}\}]_{pq}^w}{\partial \beta} = - H^w(pq) \cos\left\{\frac{\hbar}{2} \left[\frac{\overleftarrow{\partial}}{\partial q} \frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p} \frac{\overrightarrow{\partial}}{\partial q} \right]\right\} [\exp\{-\beta\hat{H}\}]_{pq}^w$$

(2.6.6a)

$$= \left[\frac{\hbar^2}{8m} \frac{\partial^2}{\partial q^2} - \frac{p^2}{2m} - V(q) \cos\left\{\frac{\hbar}{2} \left[\frac{\overleftarrow{\partial}}{\partial q} \frac{\overrightarrow{\partial}}{\partial p} \right]\right\} \right] [\exp\{-\beta\hat{H}\}]_{pq}^w$$

(2.6.6b)

where equation (2.6.6b) follows for the Hamiltonian $H^w(pq) = p^2/2m + V(q)$.

So that for a given potential we can try to solve equation (2.6.6), with the initial condition

$$[\exp\{-\beta\hat{H}\}]_{pq, \beta=0}^w = 1 \quad (2.6.7)$$

For potentials up to and including terms quadratic in q , one can use the trial function

$$[\exp\{-\beta\hat{H}\}]_{pq}^w = \exp\{-AH + B\} \quad (2.6.8)$$

where A and B are functions of β only such that $A = B = 0$ when $\beta = 0$ and H is the Hamiltonian given by equation (2.5.5), with time independent potential.

Substituting equation (2.6.8) into (2.6.6b) yields

$$\begin{aligned}
& \left[-\frac{dA}{d\beta} H + \frac{dB}{d\beta} \right] \left[\exp\{-\beta\hat{H}\} \right]_{pq}^w \\
&= -H \left[\exp\{-\beta\hat{H}\} \right]_{pq}^w + \frac{\hbar^2}{4} \left[-\frac{A}{m} \frac{\partial^2 H}{\partial q^2} + \frac{A^2}{2m} \left[\left(\frac{\partial H}{\partial q} \right)^2 + \frac{p^2}{m} \frac{\partial^2 H}{\partial q^2} \right] \right] \left[\exp\{-\beta\hat{H}\} \right]_{pq}^w \\
&= -H \left[\exp\{-\beta\hat{H}\} \right]_{pq}^w + \frac{\hbar^2}{4} \left[\frac{2A^2 a}{m} H - \frac{A}{m} \left[2a - \frac{Ab^2}{2} \right] \right] \left[\exp\{-\beta\hat{H}\} \right]_{pq}^w
\end{aligned}
\tag{2.6.9}$$

In obtaining the last expression we have assumed that the Hamiltonian has the general quadratic form with Weyl transform

$$H = \frac{p^2}{2m} + aq^2 + bq \tag{2.6.10}$$

where a and b are constants.

Rearranging equation (2.6.9), gives

$$\left[-\frac{dA}{d\beta} + 1 - \frac{\hbar^2 a}{2m} A^2 \right] H + \left[\frac{dB}{d\beta} + \frac{\hbar^2 A}{4m} \left[2a - \frac{Ab^2}{2} \right] \right] = 0
\tag{2.6.11}$$

Equation (2.6.11) must be true for all p, q hence each square bracket must be equated to zero, thus we have

$$-\frac{dA}{d\beta} - \frac{\hbar^2 a}{2m} A^2 + 1 = 0 \tag{2.6.12}$$

and

$$\frac{dB}{d\beta} + \frac{\hbar^2 A}{4m} \left[2a - \frac{Ab^2}{2} \right] = 0 \quad (2.6.13)$$

Equation (2.6.12) can be solved immediately to get

$$A(\beta) = \frac{1}{\alpha} \tanh(\alpha\beta) \quad (2.6.14)$$

where

$$\alpha = \left[\frac{\hbar^2 a}{2m} \right]^{\frac{1}{2}}$$

Substituting equation (2.6.14) into (2.6.13) and solving for B, we get

$$B(\beta) = -\ln\{\cosh(\alpha\beta)\} + \frac{b^2}{4a} \left[\frac{1}{\alpha} \tanh(\alpha\beta) - \beta \right] \quad (2.6.15)$$

Therefore, we have

$$\left[\exp\{-\beta\hat{H}\} \right]_{pq}^w = \text{sech}(\alpha\beta)$$

$$\times \exp\left\{ -\frac{H}{\alpha} \tanh(\alpha\beta) - \frac{b^2}{4a} \left[\frac{1}{\alpha} \tanh(\alpha\beta) - \beta \right] \right\} \quad (2.6.16)$$

Equation (2.6.16) is exact for these potentials. Clearly, as the potential increases from quadratic the process of producing analytical solutions becomes increasingly difficult, even impossible.

If we take the case of a simple harmonic oscillator, where

$$a = \frac{1}{2} m\omega^2 \quad \text{and} \quad b = 0$$

and insert these into equation (2.6.16), we get

$$[\exp\{-\beta\hat{H}\}]_{pq}^w = \operatorname{sech}\left[\frac{\hbar\omega\beta}{2}\right] \exp\left\{-\frac{2}{\hbar\omega} H \tanh\left[\frac{\hbar\omega\beta}{2}\right]\right\} \quad (2.6.17)$$

where

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2$$

Integration of equation (2.6.17) over p and q , yields for the partition function

$$Z = \frac{1}{2\sinh\left[\frac{\hbar\omega\beta}{2}\right]} \quad (2.6.18)$$

Taking the Weyl transform of equation (2.6.1), dividing by h and using equations (2.6.17) and (2.6.18), one obtains the Wigner function for the harmonic oscillator in thermal equilibrium, namely

$$P^W(pq) = \frac{\tanh\left[\frac{\hbar\omega\beta}{2}\right]}{\pi\hbar} \exp\left\{-\frac{2}{\hbar\omega} H \tanh\left[\frac{\hbar\omega\beta}{2}\right]\right\} \quad (2.6.19)$$

Thus, we have an alternative derivation for the thermal oscillator of Davies and Davies [28]. In addition, equation (2.6.19) is an example of a non-negative Wigner function for mixed states.

An alternative method for finding $(\exp\{-\beta\hat{H}\})_{pq}^W$ hinges on the Weyl transform of the propagator \hat{U}_t , namely

$$[\hat{U}_t]_{pq}^W = \left[\exp\left\{-\frac{i}{\hbar} \hat{H}t\right\}\right]_{pq}^W \quad (2.6.20)$$

then from equation (1.3.16) one gets

$$\left[\exp\left\{-\frac{i}{\hbar} \hat{H}t\right\}\right]_{pq}^W = \int \exp\left\{\frac{i}{\hbar} pv\right\} \left\langle q - \frac{1}{2}v \middle| \hat{U}_t \middle| q + \frac{1}{2}v \right\rangle dv \quad (2.6.21)$$

The second factor on the rhs of equation (2.6.21) is the usual Schroedinger propagator (Greens' function)

$$K\left(q - \frac{1}{2}v, t \middle| q + \frac{1}{2}v, 0\right) \quad (2.6.22)$$

so that equation (2.6.21) becomes

$$\left[\exp\left\{-\frac{i}{\hbar} \hat{H}t\right\}\right]_{pq}^W = \int \exp\left\{\frac{i}{\hbar} pv\right\} K\left(q - \frac{1}{2}v, t \middle| q + \frac{1}{2}v, 0\right) dv \quad (2.6.23)$$

Letting $t = -i\hbar\beta$ in equation (2.6.23) yields

$$\left[\exp\{-\beta\hat{H}\}\right]_{pq}^w = \int \exp\left\{\frac{i}{\hbar} pv\right\} K\left(q - \frac{1}{2}v, -i\hbar\beta \left| q + \frac{1}{2}v, 0\right.\right) dv \quad (2.6.24)$$

Hence, the Weyl transform of $\exp\{-\beta\hat{H}\}$ can be expressed in terms of the Schroedinger propagator for imaginary times.

Furthermore, for the equipartition function we have

$$Z = \text{Tr}\left[\exp\{-\beta\hat{H}\}\right] = \int K(q, -i\hbar\beta | q, 0) dv \quad (2.6.25)$$

Which shows that one can, also, get the equipartition function from the usual Schroedinger propagator for imaginary times. The properties of the kernel $K(xt|y0)$ will be discussed in Chapter 3.

CHAPTER THREE

PROPAGATORS IN PSEUDO PHASE SPACE

3.1 INTRODUCTION

In ordinary quantum mechanics, [11], we learn that the time evolution of the wave-function can be expressed in terms of an integral equation. The kernel, Greens' function or Schroedinger propagator, of this equation is the transformation function which evolves the initial wave-function to a future time and will be denoted by $K(xt|y0)$. We shall see in Section 3.2 that the kernel is a solution to the Schroedinger equation.

In the path sum formulation of quantum mechanics of Feynmann, [29], $K(xt|y0)$ is described as a probability amplitude. That is, the probability for a system to arrive at the point x at time t , in configuration space, conditional on y at time 0 , is just the absolute value squared of the amplitude. There are an infinite number of classical paths of different phases contributing during time t to the overall total amplitude, and each path has a phase that is proportional to the action S . Thus, $K(xt|y0)$ is the sum over all paths from y to x .

In symbols, one writes the following "path sum" for $K(x,t|y,0)$ as

$$K(xt|y0) = \text{const} \int_y^x \exp\left\{\frac{i}{\hbar} S(x,y)\right\} D[q(t)]$$

where $S(x,y)$ is the classical action of the corresponding classical system, which is given by

$$S(x,y) = \int_0^t L(\dot{q}(t'), q(t'), t') dt'$$

where L is the Lagrangian. The constant in the path sum is chosen so that

$K(xt|y_0) \rightarrow \delta(x - y)$ as $t \rightarrow 0$.

For a function to qualify as a propagator certain conditions and properties must be met, and these are outlined in Section 3.2. Propagators with a similar character can also be constructed in pseudo phase space. Such propagators will be written in terms of the dual space of position and momentum coordinates. This shows a formal parallel between the Wigner-Weyl and Schroedinger pictures of quantum mechanics.

There are two pseudo phase space propagators in the literature. They are the Wigner propagator, [1] [3], and the Q-propagator, [32]. The Wigner propagator, as its name suggests, connects the initial and final Wigner functions of a system and shall be defined as the kernel of the integral equation describing the time evolution of the Wigner function (cf Section 3.2). Whereas the Q-propagator, by definition, is the kernel of the integral equation describing the time development of the initial and final Weyl transforms of the evolution operator (cf Section 3.5). Both propagators are themselves Weyl transforms of products of the delta operator $\hat{\Delta}_{pq}$, evolution operator $\hat{U}(t)$ and its Hermitian conjugate.

In this Chapter we shall discuss both the Wigner and Q - propagators. In Section 3.2 the integral equation for the Wigner function is derived. Then we show how the various representations of quantum mechanics can be used to obtain different, but equivalent, expressions for the Wigner propagator. The conditional characteristic function of Moyal, [19], is then briefly discussed. In Section 3.3 we shall analyse the properties of the Wigner propagator. These properties will influence our qualitative and quantitative understanding of this propagator. In Section 3.4 we finally find its equation of motion and introduce the quantum Liouville operator. Section 3.5 introduces the Q-propagator in a style similar to that used for the Wigner propagator and alternative expressions are found. In Section 3.6 we list some of the properties of the Q-propagator. Finally, in Section 3.7

3.2 THE FORM OF THE WIGNER PROPAGATOR

In Chapter 2, we found that the Wigner function is governed, for Hamiltonian (2.5.3), by a equation of motion, equation (2.5.4) or (2.5.6). An alternative way is to express the time development from an initial Wigner function, $P^W(p_0, q_0, 0)$, to the Wigner function at time t , $P^W(p, q, t)$, where $t > 0$, by an integral equation. This integral equation can be found by first remembering that in ordinary quantum formulations the state $|\psi_t\rangle$ is propagated from an initial state $|\psi_0\rangle$ at time 0 by the unitary operator $\hat{U}(t, 0)$ as follows

$$|\psi_t\rangle = \hat{U}(t, 0)|\psi_0\rangle \quad (3.2.1a)$$

where $\hat{U}(t, 0)$ satisfies the equation

$$i\hbar \frac{\partial \hat{U}(t, 0)}{\partial t} = \hat{H}\hat{U}(t, 0) \quad (3.2.1b)$$

with the initial condition

$$\hat{U}(0, 0) = 1 \quad (3.2.1c)$$

Starting with equation (2.2.11) and using equations (3.2.1) along with equation (1.2.3) one finds that

$$P^W(p, q, t) = \frac{1}{\hbar} \langle \psi_t | \hat{\Delta}_{pq} | \psi_t \rangle$$

$$= \frac{1}{\hbar} \langle \psi_0 | \hat{U}^+(t, 0) \hat{\Delta}_{pq} \hat{U}(t, 0) | \psi_0 \rangle$$

$$= \frac{1}{\hbar^2} \iint [\hat{U}^+(t, 0) \hat{\Delta}_{pq} \hat{U}(t, 0)]_{p_0 q_0}^W \langle \psi_0 | \hat{\Delta}_{p_0 q_0} | \psi_0 \rangle dp_0 dq_0$$

$$= \int P(pqt | p_0 q_0 0) P^W(p_0 q_0 0) dp_0 dq_0 \quad (3.2.2a)$$

where we have defined

$$P(pqt | p_0 q_0 0) = \frac{1}{\hbar} [\hat{U}^+(t, 0) \hat{\Delta}_{pq} \hat{U}(t, 0)]_{p_0 q_0}^W \quad (3.2.2b)$$

as the Wigner propagator, which denotes the quasi-conditional probability of the pseudo phase points p and q at time t conditional on p_0, q_0 at time zero, and

$$P^W(p_0 q_0 0) = \frac{1}{\hbar} \langle \psi_0 | \hat{\Delta}_{p_0 q_0} | \psi_0 \rangle$$

as the initial Wigner function.

From equation (3.2.1c) and (1.3.14), we have

$$P(pq0 | p_0 q_0 0) = \delta(p - p_0) \delta(q - q_0) \quad (3.2.3)$$

as the initial condition.

The resemblance of the Wigner propagator to a classical conditional

probability distribution is only formal, since like the Wigner function, $P(pqt|p_0q_0)$ is a fully quantum mechanical object. In addition, cf Section 3.3, the Wigner propagator is not always non-negative in pseudo phase space and thus cannot be interpreted as a true conditional probability.

It is the intention of this section to find suitable expressions for $P(pqt|p_0q_0)$ which can be used in calculations. This will be achieved by applying some techniques of ordinary quantum mechanics. For convenience we shall work with a time independent Hamiltonian unless stated otherwise.

In the Schroedinger picture of quantum mechanics, [11], the time evolution of the initial wave function $\psi(y,0)$ to a later time t , $t > 0$, is given by

$$\psi(x,t) = \int K(xt|y0)\psi(y,0)dy \quad (3.2.4)$$

where the kernel, $K(xt|y0)$, of the integral equation is the Schroedinger propagator or Greens' function.

Clearly, $K(xt|y0)$ must satisfy the initial condition

$$K(x0|y0) = \delta(x - y) \quad (3.2.5)$$

The kernel $K(xt|y0)$ is a solution to the Schroedinger equation. This can be seen for instance by substituting equation (3.2.4) into (2.5.1a), to get (for time independent potentials)

$$i\hbar \frac{\partial K(xt|y0)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 K(xt|y0)}{\partial x^2} + V(x)K(xt|y0) \quad (3.2.6)$$

with the initial condition given by equation (3.2.5).

Let the Hamiltonian operator be expressed as follows:

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \quad (3.2.7)$$

Since we are assuming that \hat{H} is independent of time, we can formally solve equation (3.2.6) to get

$$K(xt|y0) = \exp\left\{-\frac{i\hat{H}t}{\hbar}\right\} \delta(x - y) \quad (3.2.8)$$

The rhs of equation (3.2.8) can be written in terms of a complete set of energy eigenfunctions $\psi_n(x)$ using

$$\delta(x - y) = \sum_n \psi_n(x) \psi_n^*(y)$$

where ψ_n is an eigenfunction of \hat{H} , then

$$K(xt|y0) = \sum_n \exp\left\{-\frac{iE_n t}{\hbar}\right\} \psi_n(x) \psi_n^*(y) \quad (3.2.9)$$

where the E_n are the energy eigenvalues satisfying the eigenvalue equation

$$\hat{H}\psi_n(x) = E_n\psi_n(x) \quad (3.2.10)$$

The Wigner propagator can be obtained in a straightforward manner, in terms of the kernel $K(xt|y0)$, by substituting equation (3.2.4) into (2.2.4) to get

$$P^W(pqt) = \frac{1}{h} \int \exp\left\{\frac{i}{h} pv\right\} K^*\left(q + \frac{1}{2} v, t|y', 0\right) K\left(q - \frac{1}{2} v, t|y, 0\right) \times \psi^*(y'0)\psi(y0)dy'dydv \quad (3.2.13)$$

Following a little manipulation we find ultimately that

$$P^W(pqt) = \int P(pqt|p_0q_00)P^W(p_0q_00)dp_0dq_0 \quad (3.2.14)$$

where we have defined the Wigner propagator as

$$P(pqt|p_0q_00) = \frac{1}{h} \int \exp\left\{\frac{i}{h}(pv - p_0v_0)\right\} K^*\left(q + \frac{1}{2} v, t|q_0 + \frac{1}{2} v_0, 0\right) \times K\left(q - \frac{1}{2} v, t|q_0 - \frac{1}{2} v_0, 0\right) dv dv_0 \quad (3.2.15)$$

and the Wigner function for state ψ is initially given by

$$P^W(p_0q_00) = \frac{1}{h} \int \exp\left\{\frac{i}{h} p_0s\right\} \psi^*\left(q_0 + \frac{1}{2} s\right) \psi\left(q_0 - \frac{1}{2} s\right) ds \quad (3.2.16)$$

We shall refer to equation (3.2.15) as the Schroedinger representation of the Wigner propagator.

A knowledge of the kernel $K(xt|y0)$ enables one, in principle, to calculate the Wigner propagator. However, there is only a short list of exact kernels available, [29b,30].

In the Heisenberg representation of quantum mechanics the time dependence is carried solely by the operators rather than by the wave-function. Thus, we have the time varying density matrix $\hat{\rho}_t$ given by

$$\hat{\rho}_t = \hat{U}(t,0)\hat{\rho}_0\hat{U}^+(t,0) \quad (3.2.17)$$

where $\hat{U}(t,0)$ is the time evolution operator (cf equation (3.2.1b)) and $\hat{U}^+(t,0)$ its Hermitian conjugate, $\hat{\rho}_0$ is the initial density matrix, and, $\hat{\rho}_t$ satisfies the equation

$$\frac{\partial \hat{\rho}_t}{\partial t} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}_t] \quad (3.2.18)$$

Taking the Weyl transform of both sides of equation (3.2.17) and using equation (1.3.15), gives

$$[\hat{\rho}_t]_{pq}^W = \text{Tr}[\hat{\Delta}_{pq}\hat{U}(t,0)\hat{\rho}_0\hat{U}^+(t,0)] \quad (3.2.19)$$

Since $\text{Tr}[\hat{A}\hat{B}] = \text{Tr}[\hat{B}\hat{A}]$ we have

$$[\hat{\rho}_t]_{pq}^W = \text{Tr}[\hat{U}^+(t,0)\hat{\Delta}_{pq}\hat{U}(t,0)\hat{\rho}_0]$$

$$= \frac{1}{\hbar} \int \left[\hat{U}^+(t,0) \hat{\Delta}_{pq} \hat{U}(t,0) \right]_{p_0 q_0}^w \left[\hat{\rho}_0 \right]_{p_0 q_0}^w dp_0 dq_0 \quad (3.2.20)$$

where we have used equation (1.3.22) in obtaining the last expression.

But

$$\left[\hat{U}^+(t,0) \hat{\Delta}_{pq} \hat{U}(t,0) \right]_{p_0 q_0}^w = \text{Tr} \left[\hat{\Delta}_{p_0 q_0} \hat{U}^+(t,0) \hat{\Delta}_{pq} \hat{U}(t,0) \right] \quad (3.2.21)$$

Dividing equation (3.2.20) by \hbar and using equation (3.2.21) gives

$$P^w(pqt) = \int P(pqt | p_0 q_0 0) P^w(p_0 q_0 0) dp_0 dq_0 \quad (3.2.22)$$

where we have defined the Wigner propagator as

$$P(pqt | p_0 q_0 0) = \frac{1}{\hbar} \text{Tr} \left[\hat{\Delta}_{pq} \hat{U}(t,0) \hat{\Delta}_{p_0 q_0} \hat{U}^+(t,0) \right] \quad (3.2.23)$$

We shall refer to equation (3.2.23) as the Heisenberg representation of the Wigner propagator. We shall show below that expression (3.2.23) for the Wigner propagator is identical to the Schrodinger representation equation (3.2.15).

We know from any standard text on quantum mechanics, [11], that there are operators, \hat{U} , which have the property that their inverse is equal to their Hermitian conjugate. Such operators are called unitary operators.

Using a unitary operation, an Hilbert space vector can be transformed into another by

$$|\varphi\rangle = \hat{U} |\psi\rangle \quad (3.2.24)$$

One can find many interesting properties resulting from unitary operators. For instance, a change of basis corresponds to a unitary transformation. The eigenvalues of an operator are invariant under a unitary transformation; so too is the expectation value. From equation (3.2.24), one can show that the magnitudes of both vectors are the same.

An important unitary operator is the time evolution operator. When the Hamiltonian is time independent, this is given by

$$\hat{U}(t,0) = \exp\left\{-\frac{i}{\hbar}\hat{H}t\right\} \quad (3.2.25)$$

where \hat{H} is the Hamiltonian operator. $\hat{U}(t,0)$ is unitary only because \hat{H} is Hermitian. $\hat{U}(t,0)$ is also unitary when \hat{H} is time -dependent, but it does not take the simple form of equation (3.2.25)). Furthermore, $\hat{U}(t,0)$ satisfies the equation (3.2.1b) and multiplying equation (3.2.1a) on the left with $\langle x|$, where $\langle x|$ represents all the coordinate eigenstates of the system, we get

$$\begin{aligned} \langle x|\psi_t\rangle &= \langle x|\hat{U}(t,0)|\psi_0\rangle \\ &= \int \langle x|\hat{U}(t,0)|y\rangle \langle y|\psi_0\rangle dy \end{aligned} \quad (3.2.29)$$

upon comparing equation (3.2.29) with (3.2.4) we can identify at once

$$K(xt|y0) = \langle x|\hat{U}(t,0)|y\rangle \quad (3.2.30)$$

Inserting equation (3.2.30) in equation (3.2.15) yields

$$P(pqt|p_0q_00) =$$

$$\frac{1}{h} \int \exp\left\{\frac{i}{h}(pv - p_0v_0)\right\} \langle q_0 + \frac{1}{2} v_0, 0 | \hat{U}^+(t,0) | q + \frac{1}{2} v, t \rangle$$

$$\times \langle q - \frac{1}{2} v, t | \hat{U}(t,0) | q_0 - \frac{1}{2} v_0, 0 \rangle dv dv_0$$

$$(3.2.31)$$

By equation (3.2.30), equation (3.2.31) is identical to the "Schroedinger form" of the Wigner propagator, equation (3.2.15).

Equations (3.2.15) or (3.2.31) and (3.2.23) are equivalent definitions for the Wigner propagator. To see that equation (3.2.23) is equivalent a little algebra is needed.

We can show this simply by substituting equation (1.3.7), for $\hat{\Delta}_{pq}$, into (3.2.23) to get

$$\begin{aligned} \frac{1}{h} \text{Tr} [\hat{\Delta}_{pq} \hat{U}(t,0) \hat{\Delta}_{p_0q_0} \hat{U}^+(t,0)] &= \frac{1}{h} \text{Tr} \left[\int \exp\left\{\frac{i}{h}(pv - p_0v_0)\right\} \right. \\ &\times \left. |q + \frac{1}{2} v\rangle \langle q - \frac{1}{2} v| \hat{U}(t,0) |q_0 + \frac{1}{2} v_0\rangle \langle q_0 - \frac{1}{2} v_0| \hat{U}^+(t,0) dv dv_0 \right] \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{\hbar} \int \exp\left\{\frac{i}{\hbar}(pv + p_0 v_0)\right\} \langle x | q + \frac{1}{2} v \rangle \\
&\times \langle q - \frac{1}{2} v | \hat{U}(t, 0) | q_0 + \frac{1}{2} v_0 \rangle \langle q_0 - \frac{1}{2} v_0 | \hat{U}^\dagger(t, 0) | x \rangle dx dv dv_0 \\
&= \frac{1}{\hbar} \int \exp\left\{\frac{i}{\hbar}(pv + p_0 v_0)\right\} \langle q - \frac{1}{2} v | \hat{U}(t, 0) | q_0 + \frac{1}{2} v_0 \rangle \\
&\times \langle q_0 - \frac{1}{2} v_0 | \hat{U}^\dagger(t, 0) | q + \frac{1}{2} v \rangle dv dv_0
\end{aligned}
\tag{3.2.32}$$

and this is the version of the propagator given in equation (3.2.31).

The criteria for preferring one definition over another can only be based on convenience. Indeed, finding exact expressions of the Wigner propagator can, usually, be quite difficult (cf Section 3.4 for an example). Also from the above definitions we see that the Wigner propagator is independent of the initial and final Wigner functions and consequently the initial and final states of the system. Thus, it behaves as a transformation function and contains information about the way in which the system evolves. Therefore, it must be dependent on the "internal" dynamics of the system.

We can express the conditional characteristic function of Moyal, [19], in terms of the Wigner propagator in the following way. The characteristic function at time $t > 0$ is given by taking the Fourier inverse of equation (2.2.12), namely

$$C_t^F(u, v) = \int \exp\left\{-\frac{i}{\hbar}(pv + qu)\right\} P^W(pqt) dp dq \tag{3.2.33}$$

Using equation (3.2.14) we get

$$\begin{aligned}
C_t^F(u, v) &= \int \exp\left\{-\frac{i}{\hbar}(pv + qu)\right\} P(pqt|p_0q_00) P^W(p_0q_00) dp dq dp_0 dq_0 \\
&= \int \exp\left\{-\frac{i}{\hbar}[(p - p_0)v + (q - q_0)u]\right\} P(pqt|p_0q_00) \\
&\quad \times \exp\left\{-\frac{i}{\hbar}(p_0v + q_0u)\right\} P^W(p_0q_00) dp dq dp_0 dq_0 \\
&= \int \exp\left\{-\frac{i}{\hbar}(p_0v + q_0u)\right\} \Lambda(pqt|p_0q_00) P^W(p_0q_00) dp dq dp_0 dq_0
\end{aligned}
\tag{3.2.34}$$

where

$$\Lambda(pqt|p_0q_00) = \int \exp\left\{-\frac{i}{\hbar}[(p - p_0)v + (q - q_0)u]\right\} P(pqt|p_0q_00) dp dq
\tag{3.2.35}$$

is the characteristic function of $p - p_0$ and $q - q_0$ conditional on p_0 and q_0 , [19].

When $t = 0$ it is evident that

$$\Lambda(pq0|p_0q_00) = 1
\tag{3.2.36}$$

3.3 PROPERTIES OF THE WIGNER PROPAGATOR

The Wigner propagator has many interesting properties, [1]. We can use these inherent properties, as we did with the Wigner function, Chapter 2 Section 2.4, to gain a meaningful understanding surrounding the existence of this propagator. In the following we shall investigate the properties of the Wigner propagator and present them in the form of a numerical list.

1) The Wigner propagator is real.

We know that $\hat{U}(t,0)$ (and hence $\hat{U}^\dagger(t,0)$) is unitary, $\hat{\Delta}_{pq}$ is Hermitian, and $P(pqt|p_0q_0,0)$ is the Weyl transform of a combination of these three operators, for instance equation (3.2.23). From the properties of the Weyl transform we infer that the Wigner propagator is real.

2) The Wigner propagator is not a Wigner function.

By equation (3.2.3), $P(pq0|p_0q_0,0)$ is a δ -function and from property 9 of Section 2.4 the Wigner function cannot be a δ -function. Thus, the Wigner propagator cannot be a Wigner function.

3) The Wigner propagator is normalized to unity.

By using any of our definitions, it is easily seen that

$$\int P(pqt|p_0q_0,0) dp dq = \int P(pqt|p_0q_0,0) dp_0 dq_0 = 1 \quad (3.3.1)$$

4) Orthogonality of the Wigner propagator.

The orthogonality of $P(pqt|p_0q_0,0)$ follows by using equation (3.2.23), (1.3.16) and (1.3.14) as

$$\int P(pqt|p_0q_0,0) P(pqt|p'_0q'_0,0) dp dq = \delta(p_0 - p'_0) \delta(q_0 - q'_0) \quad (3.3.2)$$

From equation (3.3.2) we can deduce that when $p_0 \neq p'_0$ and $q_0 \neq q'_0$ then

$$\int P(pqt|p_0q_00)P(pqt|p'_0q'_00)dpdq = 0 \quad (3.3.3a)$$

Therefore, we conclude that for the integral in equation (3.3.3a) to be zero the propagators are expected to take on negative values within the range of integration.

When $p_0 = p'_0$ and $q_0 = q'_0$ then equation (3.3.2) becomes

$$\int [P(pqt|p_0q_00)]^2 dpdq = \infty \quad (3.3.3b)$$

Equation (3.3.3b) shows that $P(pqt|p_0q_00)$ is not a square integrable function. (In Section 3.4 we shall find for potentials up to and including the harmonic oscillator that $P(pqt|p_0q_00)$ is a product of δ -functions with time dependent arguments).

To complement equation (3.3.2), we can likewise find that

$$\int P(p'q't|p_0q_00)P(pqt|p_0q_00)dp_0dq_0 = \delta(p - p')\delta(q - q') \quad (3.3.4)$$

For the remaining properties it will be convenient to introduce the initial time t_0 into equation (3.2.25) such that we have

$$\hat{U}(t, t_0) = \exp\left\{-\frac{i}{\hbar}\hat{H}(t - t_0)\right\} \quad (3.3.5)$$

5) The Wigner propagator is symmetrical with respect to exchange of position and time co-ordinates.

This can be easily seen for instance from definition (3.2.23) of $P(pqt|p_0q_0t_0)$ by interchanging the initial and final pseudo phase space variables to get (for \hat{H} time independent)

$$P(pqt|p_0q_0t_0) = P(p_0q_0t_0|pqt) \quad (3.3.6)$$

6) Time reversal property of the Wigner propagator.

This property follows by replacing t by $-t$ and t_0 by $-t_0$ any one of our definitions. (To use equation (3.2.15) it must be remembered that $K(x,t|y,t_0) = K^*(y,t_0|x,t)$). Thus time reversal of the Wigner propagator yields

$$P(pq-t|p_0q_0-t_0) = P(p_0q_0t_0|pqt_0) \quad (3.3.7)$$

This property of the Wigner propagator does not hold true for a time dependent Hamiltonian.

7) The propagation of the Wigner propagator.

The Wigner propagator follows a "Markoffian", [31], process. That is

$$P(pqt|p_0q_0t_0) = \int P(pqt|p_1q_1t_1)P(p_1q_1t_1|p_0q_0t_0)dp_1dq_1 \quad (3.3.8)$$

where $t \geq t_1 \geq t_0$.

To show this propagation property we shall substitute equation (3.2.23)

for $P(pqt|p_0q_0t_0)$ into equation (3.3.8) and use equation (1.3.22), to get

$$\begin{aligned}
& \int P(pqt|p_1q_1t_1)P(p_1q_1t_1|p_0q_0t_0)dp_1dq_1 \\
&= \frac{1}{h^2} \int \left[\hat{U}^+(t,t_1)\hat{\Delta}_{pq}\hat{U}(t,t_1) \right]_{p_1q_1}^w \left[\hat{U}(t_1,t_0)\hat{\Delta}_{p_0q_0}\hat{U}^+(t_1,t_0) \right]_{p_1q_1}^w dp_1dq_1 \\
&= \frac{1}{h} \text{Tr} \left[\hat{U}^+(t,t_1)\hat{\Delta}_{pq}\hat{U}(t,t_1)\hat{U}(t_1,t_0)\hat{\Delta}_{p_0q_0}\hat{U}^+(t_1,t_0) \right] \\
&= \frac{1}{h} \text{Tr} \left[\hat{U}^+(t,t_0)\hat{\Delta}_{pq}\hat{U}(t,t_0)\hat{\Delta}_{p_0q_0} \right] \\
&= \frac{1}{h} \text{Tr} \left[\hat{\Delta}_{pq}\hat{U}(t,t_0)\hat{\Delta}_{p_0q_0}\hat{U}^+(t,t_0) \right] \\
&= P(pqt|p_0q_0t_0) \quad (\text{by definition, equation (3.2.23)}) \quad (3.3.9)
\end{aligned}$$

By a similar argument we can show that the Wigner propagator propagates in a Markovian way even for a time dependent Hamiltonian. In that case it is still true that the law of composition holds, [11], namely

$$\hat{U}(t,t_0) = \hat{U}(t,t_1)\hat{U}(t_1,t_0) \quad (3.3.10)$$

for $t \geq t_1 \geq t_0$ and thus property (3.3.8) is proven.

By splitting the interval (t,t_0) into n small sub-intervals δt so that $t-t_0 = n\delta t$ and applying the Markovian property, equation (3.3.8),

repeatedly one finds

$$P(pqt|p_0q_0t_0) = \prod_{j=0}^{n-1} \int P(p_{j+1}q_{j+1}t_{j+1}|p_jq_jt_j) dp_{j+1} dq_{j+1} \quad (3.3.11)$$

with $p_n = p$, $q_n = q$, $t_n = t$

Equation (3.3.11) is reminiscent of the path sum formulation initiated by Feynmann, [29], for the usual quantum propagator $K(xt|y_0)$, although it is not possible to express it in terms of an action as one can for the usual propagator $K(xt|y_0)$.

3.4 TIME DEVELOPMENT OF THE WIGNER PROPAGATOR

Any object that varies in time obeys an equation of motion. The Wigner propagator is no exception. Just as $K(xt|y_0)$, the propagator for the wave-function, satisfies the Schroedinger equation so the Wigner propagator satisfies the same equation of motion as the Wigner function. This can be seen by substituting equation (3.2.2a) into (2.5.4) to get

$$\begin{aligned} \frac{\partial P_0(pqt|p_0q_0t_0)}{\partial t} &= \frac{2}{\hbar} H^W(pq) \sin \left\{ \frac{\hbar}{2} \left[\frac{\overleftarrow{\partial}}{\partial q} \frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p} \frac{\overrightarrow{\partial}}{\partial q} \right] \right\} P(pqt|p_0q_0t_0) \\ &= - L(pq) P(pqt|p_0q_0t_0) \end{aligned} \quad (3.4.1)$$

where have defined the quantum Liouville operator as

$$L(pq) = -\frac{2}{\hbar} H^W(pq) \text{Sin} \left\{ \frac{\hbar}{2} \left[\frac{\overleftarrow{\partial} \overrightarrow{\partial}}{\partial q \partial p} - \frac{\overleftarrow{\partial} \overrightarrow{\partial}}{\partial p \partial q} \right] \right\} \quad (3.4.2)$$

Alternatively, a slightly longer method would be to differentiate equation (3.2.23) with respect to time and use equation (3.3.10), (1.3.22) and (1.3.19).

Equation (3.4.1) can be solved formally with the initial condition

$$P(pqt|p_0q_0t_0) = \delta(p - p_0)\delta(q - q_0) \quad (3.4.3)$$

to give the formal solution as

$$P(pqt|p_0q_0t_0) = \exp\{-L(pq)(t - t_0)\} \delta(p - p_0)\delta(q - q_0) \quad (3.4.4)$$

For potentials up to and including the harmonic oscillator equation (3.4.4) is independent of \hbar , but the formalism is still completely quantum. This was discussed in Section 2.5 with regard to equation (2.5.7).

As an example we shall find the Wigner propagator for the harmonic oscillator. The Hamiltonian for the harmonic oscillator is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{q}^2 \hat{\rightleftharpoons} \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2 = H(pq) \quad (3.4.5)$$

Substituting equation (3.4.5) into (3.4.2), and using (3.4.1), gives

$$\frac{\partial P(pqt|p_0q_0t_0)}{\partial t} = m\omega^2 q \frac{\partial P(pqt|p_0q_0t_0)}{\partial p} - \frac{p}{m} \frac{\partial P(pqt|p_0q_0t_0)}{\partial q} \quad (3.4.6)$$

Equation (3.4.6) is the classical equation for flow in phase space, whose solution is

$$P(pqt|p_0q_0t_0) = \delta(p - p(p_0q_0t-t_0))\delta(q - q(p_0q_0t-t_0)) \quad (3.4.7)$$

where $p(p_0q_0t-t_0)$ and $q(p_0q_0t-t_0)$ are the classical harmonic oscillator solutions of Hamiltons' equations, namely

$$\frac{\partial p(p_0q_0t-t_0)}{\partial t} = -m\omega^2 q(p_0q_0t-t_0) \quad (3.4.8a)$$

and

$$\frac{\partial q(p_0q_0t-t_0)}{\partial t} = \frac{1}{m} p(p_0q_0t-t_0) \quad (3.4.8b)$$

Here p and q are expressed as functions of the initial conditions p_0 , q_0 and the time interval $t-t_0$. Such that, at $t=t_0$ we have

$$p(p_0q_00) = p_0 \quad \text{and} \quad q(p_0q_00) = q_0 \quad (3.4.9)$$

It is straightforward to show that equation (3.4.7) is solution to equation (3.4.6) as follows.

Setting $p(t) = p(p_0 q_0 t - t_0)$ and $q(t) = q(p_0 q_0 t - t_0)$ and differentiating equation (3.4.7) with respect to time gives

$$\begin{aligned}
 & \frac{\partial [\delta(p - p(t)) \delta(q - q(t))]}{\partial t} \\
 &= \frac{\partial \delta(p - p(t))}{\partial t} \delta(q - q(t)) + \delta(p - p(t)) \frac{\partial \delta(q - q(t))}{\partial t} \\
 &= -p'(t) \delta'(p - p(t)) \delta(q - q(t)) - q'(t) \delta(p - p(t)) \delta'(q - q(t)) \\
 &= m\omega^2 q(t) \frac{\partial [\delta(p - p(t)) \delta(q - q(t))]}{\partial p} - \frac{p(t)}{m} \frac{\partial [\delta(p - p(t)) \delta(q - q(t))]}{\partial q} \\
 &= m\omega^2 q \frac{\partial [\delta(p - p(t)) \delta(q - q(t))]}{\partial p} - \frac{p}{m} \frac{\partial [\delta(p - p(t)) \delta(q - q(t))]}{\partial q}
 \end{aligned}$$

where we have used equations (3.4.8).

Solving equations (3.4.8) yields

$$p(p_0 q_0 t - t_0) = p_0 \cos \omega(t - t_0) - m\omega q_0 \sin \omega(t - t_0) \quad (3.4.11a)$$

and

$$q(p_0 q_0 t - t_0) = q_0 \cos \omega(t - t_0) + \frac{p_0}{m\omega} \sin \omega(t - t_0) \quad (3.4.11b)$$

Thus, the Wigner propagator for the harmonic oscillator is, by combining equations (3.4.7) and (3.4.11)

$$P(pqt|p_0q_0t_0) = \delta(p - p_0 \cos \omega(t-t_0) + q_0 m \omega \sin \omega(t-t_0)) \\ \times \delta(q - q_0 \cos \omega(t-t_0) - \frac{p_0}{m\omega} \sin \omega(t-t_0))$$

(3.4.12)

In the classical limit, $\hbar \rightarrow 0$, the Liouville operator, equation (3.4.2) becomes

$$L^{cl}(pq) = \frac{\partial H(pq)}{\partial q} \frac{\partial}{\partial p} - \frac{\partial H(pq)}{\partial p} \frac{\partial}{\partial q}$$

(3.4.13)

and $P(pqt|p_0q_0t_0)$ becomes the classical conditional probability distribution $P^{cl}(pqt|p_0q_0t_0)$. Consequently, equation (3.4.1) reduces to the formal classical result

$$P^{cl}(pqt|p_0q_0t_0) = \exp\{L^{cl}(pq)(t-t_0)\} \delta(p - p_0) \delta(q - q_0)$$

(3.4.14)

For quadratic Hamiltonians $L = L^{cl}$ exactly, so the system evolves classically. The initial Wigner function will, of course, involve \hbar .

3.5 THE Q-PROPAGATOR

The Q-propagator was first defined and utilised by Smith, [32], in order to construct a semi-classical approximation for the Weyl transform of the evolution operator, $\hat{U}(t,0)$. As he pointed out in his paper the Q-propagator should be able to generate interesting approximations for other quantities. For instance, one such quantity is the Wigner propagator (cf equation (52) of his paper). Before we discuss the Q-propagator it will be particularly useful to adopt the notation of [32] for the Weyl transform of the evolution operator, namely

$$U(pqt) = \left[\exp \left\{ -\frac{i}{\hbar} \hat{H} t \right\} \right]_{pq}^W \quad (3.5.1)$$

By definition, the Q-propagator propagates an initial $U(pq0) = 1$ to later times, and satisfies an integral equation. We can construct this integral equation from the time development of $U(pqt)$ since the kernel is the Q-propagator (defined only for time independent Hamiltonians), as follows

$$U(pqt) = \int Q(pqt|p_0q_00) dp_0 dq_0 \quad (3.5.2)$$

where

$$Q(pqt|p_0q_00) = \frac{1}{\hbar} \text{Tr} \left[\hat{\Delta}_{pq} \hat{U}(t/2,0) \hat{\Delta}_{p_0q_0} \hat{U}(t/2,0) \right] \quad (3.5.3)$$

The value of $Q(pqt|p_0q_00)$ is that it will yield $U(pqt)$ by integration over initial co-ordinates, equation (3.5.2). It is clear from equation (3.5.3) and (1.3.14) that we have

$$Q(pq0|p_0q_00) = \delta(p - p_0)\delta(q - q_0) \quad (3.5.4)$$

as the initial condition.

Applying equation (1.3.7) to (3.5.3) we have the alternative expression

$$Q(pqt|p_0q_00) = \frac{1}{h} \int \exp\left\{\frac{i}{h}(pv + p_0v_0)\right\} \\ \times \langle q - \frac{1}{2}v | \hat{U}(t/2, 0) | q_0 + \frac{1}{2}v_0 \rangle \langle q_0 - \frac{1}{2}v_0 | \hat{U}(t/2, 0) | q + \frac{1}{2}v \rangle dv dv_0 \quad (3.5.5)$$

Finally, by using equation (3.2.30), we find that $Q(pqt|p_0q_00)$ is related to the Schroedinger kernel by

$$Q(pqt|p_0q_00) = \frac{1}{h} \int \exp\left\{\frac{i}{h}(pv + p_0v_0)\right\} \\ \times K(q - \frac{1}{2}v, t/2 | q_0 + \frac{1}{2}v_0, 0) K(q_0 - \frac{1}{2}v_0, t/2 | q + \frac{1}{2}v, 0) dv dv_0 \quad (3.5.6)$$

Equation (3.5.2) can be inverted so that the Q -propagator can be expressed in terms of $U(pqt)$. This is obtained by inserting the transformation law

$$v = v' - 2q' + (q - q_0) , \quad v_0 = v' + 2q' + (q - q_0) \quad (3.5.7)$$

into equation (3.5.5). After some algebra one arrives at

$$\begin{aligned} Q(pqt|p_0q_00) &= \frac{4}{h^2} \int U(p + p', \frac{q + q_0}{2} + q', \frac{t}{2}) \\ &\times U^*(p_0 - p', \frac{q + q_0}{2} - q', \frac{t}{2}) \exp\left\{ \frac{2i}{\hbar} [p'(q - q_0) - q'(p - p_0)] \right\} \\ &\times \exp\left\{ \frac{i}{\hbar} (p - p_0)(q - q_0) \right\} dp' dq' \end{aligned} \quad (3.5.8)$$

3.6 PROPERTIES OF THE Q-PROPAGATOR

The Q-propagator shares some of the properties of the Wigner propagator. However, it was originally devised to produce a semi-classical approximation for $U(pqt)$. We shall now present some of the properties of $Q(pqt|p_0q_00)$ in the usual form of a numerical list.

1) The Q-propagator is real.

We know that $\hat{U}(t/2, 0)$ is unitary, $\hat{\Delta}_{pq}$ is Hermitian and $Q(pqt|p_0q_00)$ is the Weyl transform of a combination of these operators, equation (3.5.3). From these properties we easily deduce that the Q-propagator is real.

2) The Q-propagator is not normalized to unity.

This property is a consequence of equation (3.5.2). Integrating $Q(pqt|p_0q_00)$ over p_0 and q_0 yields $U(pqt)$. Alternatively, integrating over p and q gives $U(p_0q_0t)$.

3) The Q-propagator is symmetrical with respect to (pq) and (p_0q_0) .

This can be seen for instance simply by interchanging the final and initial pseudo phase space variables in definition (3.5.3) to get

$$Q(pqt|p_0q_00) = Q(p_0q_0t|pq0) \quad (3.6.1)$$

4) Time reversal property of the Q-propagator.

Replacing t by $-t$ in equation (3.5.3) gives

$$Q(pq-t|p_0q_00) = \frac{1}{\hbar} \text{Tr} [\hat{\Delta}_{pq} \hat{U}(-t/2, 0) \hat{\Delta}_{p_0q_0} \hat{U}(-t/2, 0)] \quad (3.6.2)$$

Therefore, time reversal is just the definition of $Q(pqt|p_0q_0t_0)$, equation (3.5.2), for negative times.

5) The propagation of the Q-propagator.

The Q-propagator follows a "Markoffian" process. That is

$$Q(pqt|p_0q_0t_0) = \int Q(pqt|p_1q_1t_1) Q(p_1q_1t_1|p_0q_0t_0) dp_1 dq_1 \quad (3.6.3)$$

This property can be shown by substituting definition (3.5.3) for $Q(pqt|p_0q_0t_0)$ and using equation (1.3.22), to get

$$\begin{aligned} & \int Q(pqt|p_1q_1t_1) Q(p_1q_1t_1|p_0q_0t_0) dp_1 dq_1 \\ &= \frac{1}{\hbar^2} \int \left[\hat{U}\left(\frac{t}{2}, \frac{t_1}{2}\right) \hat{\Delta}_{pq} \hat{U}\left(\frac{t}{2}, \frac{t_1}{2}\right) \right]_{p_1q_1}^w \left[\hat{U}\left(\frac{t_1}{2}, \frac{t_0}{2}\right) \hat{\Delta}_{p_0q_0} \hat{U}\left(\frac{t_1}{2}, \frac{t_0}{2}\right) \right]_{p_1q_1}^w dp_1 dq_1 \\ &= \frac{1}{\hbar} \text{Tr} \left[\hat{U}\left(\frac{t}{2}, \frac{t_1}{2}\right) \hat{\Delta}_{pq} \hat{U}\left(\frac{t}{2}, \frac{t_1}{2}\right) \hat{U}\left(\frac{t_1}{2}, \frac{t_0}{2}\right) \hat{\Delta}_{p_0q_0} \hat{U}\left(\frac{t_1}{2}, \frac{t_0}{2}\right) \right] \end{aligned}$$

$$= \frac{1}{\hbar} \text{Tr} \left[\hat{\Delta}_{pq} \hat{U}(\frac{t}{2}, \frac{t_0}{2}) \hat{\Delta}_{p_0 q_0} \hat{U}(\frac{t}{2}, \frac{t_0}{2}) \right]$$

$$= Q(pqt|p_0 q_0 t_0) \quad \text{by definition} \quad (3.6.4)$$

Equation (3.6.3) can be generalized for infinitesimal time intervals just as for equation (3.3.11) to obtain

$$Q(pqt|p_0 q_0 t_0) = \overline{\prod_{j=0}^{n-1}} \int Q(p_{j+1}, q_{j+1}, t_{j+1} | p_j, q_j, t_j) dp_{j+1} dq_{j+1} \quad (3.6.5)$$

where $t = t_n$.

As we have mentioned $Q(pqt|p_0 q_0 t_0)$ has not been defined for time dependent Hamiltonians. For the case $\hat{H}(t)$ we have the situation

$$\hat{U}(\frac{t}{2}, \frac{t_0}{2}) \hat{U}(\frac{t}{2}, \frac{t_0}{2}) \neq \hat{U}(t, t_0) \quad (3.6.6)$$

and thus $Q(pqt|p_0 q_0 t_0)$ does not propagate for time dependent Hamiltonians.

3.7 TIME DEVELOPMENT OF THE Q-PROPAGATOR

The equation of motion for the Q-propagator can be readily obtained by differentiating equation (3.5.3) with respect to time. Thus

$$\begin{aligned}
\frac{\partial Q(pqt|p_0q_0,0)}{\partial t} &= \frac{1}{\hbar} \text{Tr} \left[\hat{\Delta}_{pq} \frac{\partial \hat{U}(t/2,0)}{\partial t} \hat{\Delta}_{p_0q_0} \hat{U}(t/2,0) \right. \\
&\quad \left. + \hat{\Delta}_{pq} \hat{U}(t/2,0) \hat{\Delta}_{p_0q_0} \frac{\partial \hat{U}(t/2,0)}{\partial t} \right] \\
&= - \frac{i}{2\hbar} \left\{ \hat{H}, \hat{U}(t/2,0) \hat{\Delta}_{p_0q_0} \hat{U}(t/2,0) \right\}_{pq}^W \quad (3.7.1)
\end{aligned}$$

Note that equation (3.7.1) is only true when \hat{H} is a constant and consequently $\hat{U}(t/2,0)$ commutes with \hat{H} .

The bracketed expression in equation (3.7.1) is the anti-commutator and its Weyl transform is the real part of equation (1.3.19). Therefore

$$\begin{aligned}
\frac{\partial Q(pqt|p_0q_0,0)}{\partial t} &= H(pq) \cos \left\{ \frac{\hbar}{2} \left[\frac{\overleftarrow{\partial}}{\partial q} \frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p} \frac{\overrightarrow{\partial}}{\partial q} \right] \right\} Q(pqt|p_0q_0,0) \\
&= \left[\frac{\hbar^2}{8m} \frac{\partial^2}{\partial p^2} - \frac{p^2}{2m} - V(q) \cos \left\{ \frac{\hbar}{2} \left[\frac{\overleftarrow{\partial}}{\partial q} \frac{\overrightarrow{\partial}}{\partial p} \right] \right\} \right] Q(pqt|p_0q_0,0) \quad (3.7.2)
\end{aligned}$$

Since

$$H(pq) = \frac{p^2}{2m} + V(q) \quad (3.7.3)$$

In principle, it is possible to find $Q(pqt|p_0q_0,0)$ by solving equation

(3.7.2) directly and using the initial condition,

$$Q(pq0|p_0q_00) = \delta(p - p_0)\delta(q - q_0) \quad (3.7.4)$$

However, obtaining analytical solutions can be very difficult, therefore it may be more practical to calculate $Q(pqt|p_0q_00)$ direct from its definitions. For potentials up to and including the harmonic oscillator the expressions for $Q(pqt|p_0q_00)$ are exact.

As an example we shall find the Q-propagator for the harmonic oscillator by using equation (3.5.6). The kernel for the harmonic oscillator is given by, [29b],

$$K(xt|y0) = \left[\frac{m\omega}{2\pi i \hbar \sin(\omega t)} \right]^{\frac{1}{2}} \exp \left\{ \frac{im\omega}{2\hbar \sin(\omega t)} \left[(x^2 + y^2) \cos(\omega t) - 2xy \right] \right\} \quad (3.7.5)$$

Substituting equation (3.7.5) into (3.5.6) gives

$$\begin{aligned} Q(pqt|p_0q_00) &= \frac{m\omega}{i\hbar^2 \sin(\omega t/2)} \int \exp \left\{ \frac{i}{\hbar} (pv + p_0v_0) \right\} \exp \left\{ \frac{im\omega}{2\hbar \sin(\omega t/2)} \right. \\ &\quad \times \left[\left((q - \frac{1}{2}v)^2 + (q_0 + \frac{1}{2}v_0)^2 + (q_0 - \frac{1}{2}v)^2 + (q + \frac{1}{2}v)^2 \right) \cos(\omega t/2) \right. \\ &\quad \left. \left. - 2 \left[(q - \frac{1}{2}v)(q_0 + \frac{1}{2}v_0) + (q_0 - \frac{1}{2}v_0)(q + \frac{1}{2}v) \right] \right] \right\} dv dv_0 \end{aligned} \quad (3.7.6)$$

Evaluating the Gaussian integrals gives, after some algebra

$$\begin{aligned}
 Q(pqt|p_0q_0) &= F(t) \exp \left\{ \frac{im\omega}{\hbar \sin(\omega t/2)} \left[(q^2 + q_0^2) \cos(\omega t/2) - 2qq_0 \right] \right\} \\
 &\times \exp \left\{ \frac{i}{\hbar m \omega \sin(\omega t/2)} \left[(p^2 + p_0^2) \cos(\omega t/2) - 2pp_0 \right] \right\}
 \end{aligned}
 \tag{3.7.7}$$

where

$$F(t) = \frac{1}{\pi i \hbar \sin(\omega t/2)}
 \tag{3.7.8}$$

CHAPTER FOUR

THE GENERALISED CORRESPONDENCE RULE

4.1 INTRODUCTION

The Wigner-Weyl picture of quantum mechanics, [19], has been the central theme of our investigation of pseudo phase space. The objective of this chapter is to examine a method for constructing a general correspondence rule and subsequently a generalised transform. This would then provide a means for obtaining alternative rules of association. Joint probability distribution functions in pseudo phase space are a result of applying a correspondence rule to the density matrix, $\hat{\rho}$. Each distribution function displays its distinctive mathematical form and unique properties. These peculiarities range from being complex functions to becoming negative (or imaginary) in some regions of pseudo phase space. It is because of these peculiarities that the various distribution functions are called "quasi" probability functions. However, attempts have been made to find a distribution function, $F(pq)$, that satisfies simultaneously the following three conditions:

$$\text{i) } F(pq) = \text{Tr}(\hat{\rho}\hat{\Omega}_{pq}) \quad (4.1.1)$$

where $\hat{\Omega}_{pq}$ is some Hermitian operator.

$$\text{ii) } F(pq) \geq 0 \quad (4.1.2)$$

that is, F is non-negative for p, q .

$$\text{iii) } \int F(pq) dp = \langle q | \hat{\rho} | q \rangle \quad (4.1.3a)$$

$$\int F(pq) dq = \langle p | \hat{\rho} | p \rangle \quad (4.1.3b)$$

that is , F produces the correct quantum marginals.

We know however from Wigner, [26] and Section 2.4 property 10, that F cannot simultaneously satisfy all three conditions.

In previous chapters we have studied in detail the simplest distribution of all, the Wigner function. Mehta, [33], carries out a review of different pseudo phase space distributions that stem from the various correspondence rules. He concludes by remarking that the characteristic qualities of pseudo phase space distributions, and their dynamics, are a direct consequence of the correspondence rule adopted between the quantum operators and classical functions. We shall see in Section 4.3 that this is indeed the case.

Cohen, [6], found that all known, and many more, quasi-distribution functions are special cases of a single generalised distribution function. The generalisation is characterised by a complex weighting function, $f(u/\hbar, v/\hbar)$. The Cohen function is given by, equation (1.5) ref [6], as

$$F(pq;f) = \frac{1}{\hbar^2} \int \exp\left\{\frac{i}{\hbar} p v\right\} \exp\left\{\frac{i}{\hbar} (q - q') u\right\} f(u/\hbar, v/\hbar) \\ \times \Psi^*(q' - \frac{1}{2} v) \Psi(q' + \frac{1}{2} v) du dv dq' \quad (4.1.4)$$

Clearly, when $f=1$ we immediately recover the Wigner function (equation (2.2.4)). Different distributions functions are produced by specifying different functions f . That is, f acts as a generator for the various distribution functions. But f intrinsically offers a much more interesting attribute. It can identify the characteristic qualities of a distribution function (or, as we shall see in Section 4.3, the rule of association). We shall demonstrate this, in Section 4.3, by deducing what conditions f must satisfy in order that $F(pq;f)$ have certain reasonable properties. The Cohen

function can be regarded as the master quasi-probability distribution function from which others are the special cases. However, they still retain the prefix "quasi" because they can take negative values and therefore are not true probability distributions.

Indeed, there are in existence non-negative distribution functions. One such function was considered by Husimi, [34], (and later by Cartwright [35] using a similar method), who smoothed the Wigner function with a minimum uncertainty wave packet. The smoothed Wigner or Husimi function does not produce the correct marginals. This is a consequence of "a proof" given by Wigner, [26]. It is possible to generate, from the Cohen function an infinite class of distribution functions that are non-negative for all p, q and produce the correct marginals. This is done by allowing f to be dependent upon the wave-function, [36]. These functions do not contradict Wigners' proof as they are not bilinear in the wave-function.

The use of generalised distribution functions other than Wigners' function is limited for practical applications. Their mathematical form is usually too cumbersome. Considerable effort has been mounted to show this rigorously. Generally, authors show that the only sensible function to use is that for which $f=1$, ie the Wigner function, [14] [39] [40].

In this chapter we shall generalise our description of pseudo phase space by following the prescription initiated by Cohen, [6]. This will be done by constructing a generalised correspondence rule and subsequently introducing the concept of a generalised transform of an operator. Several suggested rules of association in past literature, [5], are then special cases of this generalised rule. The generating function f takes a specific form for each of the correspondence rules.

In Section 4.2 we devise a generalised correspondence rule. Section 4.3 establishes the criteria met by f which determines the characteristic properties of the rules of association. We then complete the generalised

correspondence rule by finding the generalised transform. In Section 4.4 we display forms of f that generate some of the more common rules. From the conditions that this f satisfies we can predict the properties of the respective rule of association. Finally, in Section 4.5 we discuss some alternatives to the Wigner function and find their equation of motion.

4.2 DEVISING A GENERALISED CORRESPONDENCE RULE

The Weyl correspondence rule, equations (1.2.3) and (1.3.15), is just one of many rules of association that have emerged since the development of quantum mechanics. It is the preferred rule for practical applications since it is the simplest. In this section we shall discuss how the other well known rules of association, [5], can be incorporated into the pseudo phase space theory we have developed so far. To do this we shall extend the concepts of Section 1.2 to devise a scheme for obtaining a generalised correspondence rule. In fact, the correspondence rule will be so general that it will enable us to construct rules of association at will. The previously mentioned rules, [5], being particular cases. The approach adopted will be closely related to that of Cohen, [6]. (Ultimately we shall then be able to appreciate how simple Weyls' rule really is).

In Section 1.2 we represented the Weyl transform, $A^W(pq)$, as a Fourier integral. In a like manner, we shall write the generalised transform, $A^f(pq)$, as

$$A^f(pq) = \int \alpha(u,v) \exp\left\{-\frac{i}{\hbar}(qu + pv)\right\} du dv \quad (4.2.1)$$

If we take as our process of quantisation the view that p and q can be, as usual, replaced by their operator equivalents and, in addition, introduce an arbitrary, and in general, complex function $f(u/\hbar, v/\hbar)$, then equation (4.2.1) becomes

$$\hat{A} = \int \alpha(u,v) f(u/\hbar, v/\hbar) \exp\left\{-\frac{i}{\hbar}(\hat{q}u + \hat{p}v)\right\} du dv \quad (4.2.2)$$

where \hat{A} is the operator corresponding to the pseudo phase space function $A^f(pq)$ and $f(u/\hbar, v/\hbar)$ is assumed to be expandable in a power series, such that

$$f(u/\hbar, v/\hbar) = \sum_{m,n} a_{mn} \frac{u^m v^n}{\hbar^{m+n}} \quad (4.2.3)$$

Eliminating $\alpha(u, v)$ from equations (4.2.1) and (4.2.2) gives (cf equation (1.2.3))

$$\hat{A} = \frac{1}{\hbar} \int A^f(pq) \hat{\Delta}_{pqf} dp dq \quad (4.2.4)$$

where the generalised delta operator is defined (cf equation (1.2.4)) by

$$\hat{\Delta}_{pqf} = \frac{1}{\hbar} \int f(u/\hbar, v/\hbar) \exp\left\{\frac{i}{\hbar}[(q - \hat{q})u + (p - \hat{p})v]\right\} du dv \quad (4.2.5)$$

or, by using equation (4.2.3), more succinctly as

$$\hat{\Delta}_{pqf} = f\left[\frac{1}{i}\frac{\partial}{\partial q}, \frac{1}{i}\frac{\partial}{\partial p}\right] \hat{\Delta}_{pq} \quad (4.2.6)$$

and $A^f(pq)$ is the generalised transform of the operator \hat{A} .

Generalised transforms, $A^f(pq)$, are essentially complex functions, (cf equation (4.3.11)), on pseudo phase space and therefore are not identical to the classical function $A^{cl}(pq)$. Only in the classical limit when, $\hbar \rightarrow 0$,

does $A^f(pq)$ become equivalent to $A^{cl}(pq)$ and therefore we must insist that the classical limit condition for f is

$$\lim_{\hbar \rightarrow 0} f(u/\hbar, v/\hbar) = 1 \quad (4.2.7)$$

The generalised correspondence rule is specified by the choice of the function $f(u/\hbar, v/\hbar)$. Hence, one can construct correspondence rules in an arbitrary fashion simply by choosing a particular f . However, selection of f is not entirely open but can be guided by imposing certain reasonable conditions which assist in reducing the choice of f . This point will be discussed in the next section. (Incidentally for the case $f=1$ one instantly recovers the Weyl correspondence rule).

4.3 INVERTING THE GENERALISED CORRESPONDENCE

The function $f(u/\hbar, v/\hbar)$ being a complex function is a member of a broad spectrum of functions. However, the choice of f can be greatly reduced by insisting that f satisfies certain reasonable conditions. These conditions are by no means mandatory. But are offered as options that assist in determining the properties governing the correspondence rule and, to some extent simplifying calculations. Therefore, to establish these conditions one must decide upon what properties the resulting correspondence rule is to exhibit.

From equation (4.2.3) we can set, without loss of any generality,

$$f(0,0) = \text{const} = 1 \quad (4.3.1)$$

Further conditions on f can be obtained from the generalised delta operator, equation (4.2.5). It is tenable to assume that $\hat{\Delta}_{pqf}$ should display properties similar to those of $\hat{\Delta}_{pq}$. Therefore, we shall demand that the generalised correspondence rule should form a complete basis for the family of linear operators. Thus, following from equations (1.3.11), (1.3.12a) and (1.3.12b) and using equation (4.2.5), we require that

$$\frac{1}{h} \int \hat{\Delta}_{pqf} dp = |q\rangle\langle q| \quad (4.3.2)$$

and

$$\frac{1}{h} \int \hat{\Delta}_{pqf} dq = |p\rangle\langle p| \quad (4.3.3)$$

Equations (4.3.2) and (4.3.3) will only be true when

$$f(0, v/h) = f(u/h, 0) = 1 \quad (4.3.4)$$

As a consequence of equations (4.3.2) to (4.3.4) and analogous to equation (1.3.13) we have

$$\frac{1}{h} \int \hat{\Delta}_{pqf} dp dq = 1 \quad (4.3.5)$$

In addition, we may require that $\hat{\Delta}_{pqf}$ should be an Hermitian operator. This ensures firstly that when \hat{A} is an Hermitian operator then $A^f(pq)$ is a real function in pseudo phase space and secondly that the correspondence

rule will produce a one-one mapping between quantum operators and classical functions. This second consequence can be seen as follows:

The Hermitian conjugate of equation (4.2.4), upon requiring $A^f(pq)$ to be real is given by

$$\hat{A} = \frac{1}{h} \int A^f(pq) \hat{\Delta}_{pqf}^+ dp dq \quad (4.3.6)$$

But if $\hat{\Delta}_{pqf}$ is not Hermitian then equation (4.3.6) is different to equation (4.2.4). Therefore, we have established that there exists two different rules of association corresponding to the same operator. Hence, we are led to the conclusion that if $\hat{\Delta}_{pqf}$ is not Hermitian then the resulting rule of association will not be a one-one mapping.

From equation (4.2.5), it follows that $\hat{\Delta}_{pqf}$ is Hermitian if

$$f^*(u/\hbar, v/\hbar) = f(-u/\hbar, -v/\hbar) \quad (4.3.7)$$

By using expression (1.3.7) for $\hat{\Delta}_{pq}$ in equation (4.2.6), $\hat{\Delta}_{pqf}$ can be written as

$$\begin{aligned} \hat{\Delta}_{pqf} &= f \left[\frac{1}{i} \frac{\partial}{\partial q}, \frac{1}{i} \frac{\partial}{\partial p} \right] \int \exp \left\{ \frac{i}{\hbar} p v \right\} \left| q + \frac{1}{2} v \right\rangle \langle q - \frac{1}{2} v | dv \\ &= \frac{1}{h} \int \exp \left\{ \frac{i}{\hbar} p v \right\} \exp \left\{ \frac{i}{\hbar} (q - q') u \right\} f(u/\hbar, v/\hbar) \\ &\quad \times \left| q' + \frac{1}{2} v \right\rangle \langle q' - \frac{1}{2} v | du dv dq' \end{aligned} \quad (4.3.8)$$

It readily follows from equation (4.3.8) that

$$\text{Tr}[\hat{\Delta}_{pqf}] = 1 \quad (4.3.9)$$

where we have used equation (4.3.4).

The trace of a product of generalised delta operators is, from equation (4.3.8),

$$\begin{aligned} \text{Tr}[\hat{\Delta}_{pqf}\hat{\Delta}_{p'q'f}] &= hf \left[\frac{1}{i} \frac{\partial}{\partial q}, \frac{1}{i} \frac{\partial}{\partial p} \right] f \left[i \frac{\partial}{\partial q}, i \frac{\partial}{\partial p} \right] \\ &\quad \times \delta(p - p') \delta(q - q') \end{aligned} \quad (4.3.10)$$

as compared to equation (1.3.14) in the Wigner-Weyl scheme.

Multiplying equation (4.2.4) on the right by $\hat{\Delta}_{pqf}$ and taking the trace of both sides yields, after using equation (4.3.10) and integrating by parts,

$$A^f(pq) = f^{-1} \left[\frac{1}{i} \frac{\partial}{\partial q}, \frac{1}{i} \frac{\partial}{\partial p} \right] f^{-1} \left[i \frac{\partial}{\partial q}, i \frac{\partial}{\partial p} \right] \text{Tr}[\hat{A}\hat{\Delta}_{pqf}] \quad (4.3.11)$$

where we have denoted $1/f$ by f^{-1} .

Equations (4.2.4) and (4.3.11) complete the generalised correspondence rule. It associates in an invertible way a function $A^f(pq)$ on pseudo phase space with an operator \hat{A} .

An alternative expression for $A^f(pq)$ can be found by using equation

(4.3.8) to get

$$\text{Tr} [\hat{A} \hat{\Delta}_{pq} f] = \frac{1}{h} \int \exp \left\{ \frac{i}{h} p v \right\} \exp \left\{ \frac{i}{h} (q - q') u \right\} f(u/h, v/h) \\ \times \left\langle q' - \frac{1}{2} v | \hat{A} | q' + \frac{1}{2} v \right\rangle du dv dq' \quad (4.3.12)$$

and substituting equation (4.3.12) into (4.3.11), gives

$$A^f(pq) = f^{-1} \left[\frac{1}{i} \frac{\partial}{\partial q}, \frac{1}{i} \frac{\partial}{\partial p} \right] f^{-1} \left[i \frac{\partial}{\partial q}, i \frac{\partial}{\partial p} \right] \frac{1}{h} \int \exp \left\{ \frac{i}{h} p v \right\} \exp \left\{ \frac{i}{h} (q - q') \right\} \\ \times f(u/h, v/h) \left\langle q' - \frac{1}{2} v | \hat{A} | q' + \frac{1}{2} v \right\rangle du dv dq' \\ = f^{-1} \left[i \frac{\partial}{\partial q}, i \frac{\partial}{\partial p} \right] \int \exp \left\{ \frac{i}{h} p v \right\} \left\langle q - \frac{1}{2} v | \hat{A} | q + \frac{1}{2} v \right\rangle dv \quad (4.3.13)$$

Recognising that the integral on the rhs of equation (4.3.13) is just the Weyl transform of \hat{A} enables us to write

$$A^f(pq) = f^{-1} \left[i \frac{\partial}{\partial q}, i \frac{\partial}{\partial p} \right] A^W(pq) \quad (4.3.14)$$

Alternatively, equation (4.3.14) follows directly from equation (4.3.11) with equations (4.2.6) and (1.3.15).

Equation (4.3.8) can be expressed in terms of momentum variables as

$$\hat{\Delta}_{pqf} = \frac{1}{h} \int \exp\left\{\frac{i}{h} qu\right\} \exp\left\{\frac{i}{h}(p - p')\right\} f(-u/h, -v/h)$$

$$x|p' - \frac{1}{2} v\rangle\langle p' + \frac{1}{2} v| du dv dp' \quad (4.3.15)$$

Substituting equation (4.3.13) and (4.3.15) into the rhs of equation (4.2.4) and transforming variables with

$$q' = q - \frac{1}{2} v, \quad q'' = q + \frac{1}{2} v, \quad p' = p - \frac{1}{2} u, \quad p'' = p + \frac{1}{2} u \quad (4.3.16)$$

one obtains

$$\int |p'\rangle\langle p'| q'\rangle\langle q'| \hat{A} |q''\rangle\langle q''| p''\rangle\langle p''| dp' dp'' dq' dq'' = \hat{A} \quad (4.3.17)$$

Thus, by using equation (4.3.13) for $A^f(pq)$ and equation (4.3.15) for $\hat{\Delta}_{pqf}$, we have established the consistency of the formalism.

If it is required that the generalised transform is to be written as

$$A^f(pq) = \text{Tr} [\hat{A} \hat{\Delta}_{pqf}] \quad (4.3.18)$$

then, from equation (4.3.11), the condition

$$f(u/h, v/h) f(-u/h, -v/h) = 1 \quad (4.3.19)$$

must be satisfied by f .

Only when equation (4.3.19) is satisfied can we write equation (4.3.13) or equation (4.3.11) with (4.3.18) as

$$A^f(pq) = f\left[\frac{1}{i}\frac{\partial}{\partial q}, \frac{1}{i}\frac{\partial}{\partial p}\right] A^w(pq) \quad (4.3.20)$$

For ease of reference table 1 lists the criteria that we have chosen to require of $\hat{\Delta}_{pqf}$ and their motivations.

i	$f(0,0) = 1$	Constant term of power series
ii	$f(0,v/\hbar) = f(u/\hbar,0) = 1$	$\hat{\Delta}_{pqf}$ should form a complete basis for the set of linear operators, eqs. (4.3.2 & 3)
iii	$f^*(u/\hbar,v/\hbar) = f(-u/\hbar,-v/\hbar)$	$\hat{\Delta}_{pqf}$ be Hermitian
iv	$f(u/\hbar,v/\hbar)f(-u/\hbar,-v/\hbar) = 1$	For the generalised transform to be written as $A^f(pq) = \text{Tr}(\hat{A}\hat{\Delta}_{pqf})$
v	$\lim_{\hbar \rightarrow 0} f(u/\hbar,v/\hbar) = 1$	Classical limit

Table 1

Allowing f to satisfy all the conditions of table 1 one finds from equations (4.2.4), (4.3.9) and (4.3.10) that, (cf equation (1.3.21)),

$$\text{Tr}[\hat{A}] = \frac{1}{\hbar} \int A^f(pq) dp dq \quad (4.3.21)$$

and, (cf equation (1.3.22)),

$$\text{Tr}[\hat{A}\hat{B}] = \frac{1}{h} \int A^f(pq)B^f(pq)dpdq \quad (4.3.22)$$

The generalised correspondence which determines the product $\hat{A}\hat{B}$ is given, using equation (4.2.4), by

$$\hat{A}\hat{B} = \frac{1}{h^2} \int A^f(pq)B^f(p'q')\hat{\Delta}_{pqf}\hat{\Delta}_{p'q'f}dpdp'dqdq' \quad (4.3.23)$$

In order to find the generalised transform of the product $\hat{A}\hat{B}$ one must first calculate $\hat{\Delta}_{pqf}\hat{\Delta}_{p'q'f}$. Following the procedure of Section 1.3 and applying the criteria of table 1 to f one finds, after some algebra, that

$$\begin{aligned} \hat{\Delta}_{pqf}\hat{\Delta}_{p'q'f} = & hf \left[\frac{1}{i} \frac{\partial}{\partial q}, \frac{1}{i} \frac{\partial}{\partial p} \right] f \left[\frac{1}{i} \frac{\partial}{\partial q'}, \frac{1}{i} \frac{\partial}{\partial p'} \right] \\ & \times f \left[i \frac{\partial}{\partial q} + i \frac{\partial}{\partial q'}, i \frac{\partial}{\partial p} + i \frac{\partial}{\partial p'} \right] \exp \left\{ \frac{i\hbar}{2} \left[\frac{\partial}{\partial q} \frac{\partial}{\partial p'} - \frac{\partial}{\partial p} \frac{\partial}{\partial q'} \right] \right\} \\ & \times \delta(p - p')\delta(q - q')\hat{\Delta}_{pqf} \end{aligned} \quad (4.3.24)$$

Substituting equation (4.3.24) into (4.3.23) and comparing the result with equation (4.2.4) one finally arrives (cf equation (1.3.19)) at

$$\begin{aligned}
[\hat{A}\hat{B}]_{pq}^f &= f \left[\frac{1}{i} \frac{\partial}{\partial q_A}, \frac{1}{i} \frac{\partial}{\partial p_A} \right] f \left[\frac{1}{i} \frac{\partial}{\partial q_B}, \frac{1}{i} \frac{\partial}{\partial p_B} \right] f \left[i \frac{\partial}{\partial q_A} + i \frac{\partial}{\partial q_B}, i \frac{\partial}{\partial p_A} + i \frac{\partial}{\partial p_B} \right] \\
&\times \exp \left\{ \frac{i\hbar}{2} \left[\frac{\partial}{\partial q_A} \frac{\partial}{\partial p_B} - \frac{\partial}{\partial p_A} \frac{\partial}{\partial q_B} \right] \right\} A^f(pq) B^f(pq) \quad (4.3.25)
\end{aligned}$$

Equation (4.3.25) indicates the complicated nature of the generalised correspondence rule even when all of the conditions of table 1 have been imposed upon f .

Having completed the generalised correspondence rule it is now clear that the Wigner-Weyl picture, $f=1$, provides by far the simplest rule of association. It is therefore the rule most suitable for practical applications.

4.4 GENERATING CORRESPONDENCE RULES

In Sections 4.2 and 4.3 we have devised a scheme that can, in principle, enable one to generate, by choosing different functions f , correspondence rules at will. The choice of f can be guided by the criteria we have arrived at as "reasonable" listed in table 1. But it is actually not necessary that f should satisfy a condition in table 1 for one to obtain a possible rule of association. In fact, most of the sample rules to be discussed below do not satisfy all our criteria for f .

The standard ordering, von Neumann, rule states that any classical function, $A^s(pq)$, must be arranged such that the q factors precede the p and then replaced with their respective operators. In symbols we can write

$$\begin{aligned}
\hat{A} &= \int A^S(qp) \delta(q - \hat{q}) \delta(p - \hat{p}) dp dq \\
&= \frac{1}{h^2} \int A^S(qp) \exp\left\{\frac{i}{h}(q - \hat{q})u\right\} \exp\left\{\frac{i}{h}(p - \hat{p})v\right\} du dv dp dq \\
&= \frac{1}{h^2} \int A^S(qp) \exp\left\{\frac{iuv}{2h}\right\} \exp\left\{\frac{i}{h}[(q - \hat{q})u + (p - \hat{p})v]\right\} du dv dp dq
\end{aligned}
\tag{4.4.1}$$

where we have used the BCH Theorem, equation (1.3.1), to get the last expression.

Comparing equation (4.4.1) with (4.2.4) we can identify the generator for the standard ordering rule as

$$f(u/h, v/h) = \exp\left\{\frac{iuv}{2h}\right\} \tag{4.4.2}$$

Clearly, equation (4.4.2) only satisfies conditions (i), (ii) and (v). Since this f fails to meet criterion (iii), the Hermiticity of $\hat{\Delta}_{pqf}$, the standard ordering rule is not a one-one mapping between quantum operators and classical functions. This was discussed by Shewell, [5].

The anti-standard ordering rule is similar to the standard ordering rule except the p factors precede the q . Following the above argument leads us to

$$f(u/h, v/h) = \exp\left[-\frac{iuv}{2h}\right] \tag{4.4.3}$$

Equation (4.4.3) is just the complex conjugate of equation (4.4.2) and satisfies the same conditions. The resulting correspondence rule, like the standard ordering rule, does not produce a one-one mapping between quantum operators and classical functions.

As we have already established Weyls' rule of association corresponds to the choice

$$f(u/\hbar, v/\hbar) = 1 \quad (4.4.4)$$

It is the simplest correspondence rule that satisfies all the criteria set down in table 1.

As a final example we shall take Riviers' rule. This is an extension of Weyls' rule and is given by, [5],

$$\begin{aligned} A &= \int A^R(pq) \frac{1}{2} (1 + \exp\{\frac{iuv}{\hbar}\}) \delta(q - \hat{q}) \delta(p - \hat{p}) dp dq \\ &= \frac{1}{\hbar^2} \int A^R(pq) \frac{1}{2} (1 + \exp\{\frac{iuv}{\hbar}\}) \exp\{\frac{i}{\hbar}(q - \hat{q})u\} \exp\{\frac{i}{\hbar}(p - \hat{p})v\} \\ &\quad \times du dv dp dq \\ &= \frac{1}{\hbar^2} \int A^R(pq) \cos\left[\frac{uv}{2\hbar}\right] \exp\left\{\frac{i}{\hbar}[(q - \hat{q})u + (p - \hat{p})v]\right\} du dv dp dq \end{aligned} \quad (4.4.6)$$

and comparing with equation (4.2.4) gives

$$f(u/\hbar, v/\hbar) = \cos\left[\frac{uv}{2\hbar}\right] \quad (4.4.7)$$

Equation (4.4.7) satisfies conditions (i) to (iii) but fails condition (iv). Since condition (iii) is satisfied Riviers' rule is a one-one mapping between quantum operators and classical functions. However, since it violates condition (iv) the Rivier transform cannot be written in the form of equation (4.3.20).

Correspondence Rule	$f(u/\hbar, v/\hbar)$	Criteria satisfied
Anti-normal	$\exp\left\{-\frac{1}{4\hbar}(u^2 + v^2)\right\}$	i, iii, v
Anti-standard	$\exp\left\{-\frac{iuv}{2\hbar}\right\}$	i, ii, v
Born-Jordan	$\frac{\sin\left\{\frac{uv}{2\hbar}\right\}}{\frac{uv}{2\hbar}}$	i, ii, iii, v
Normal	$\exp\left\{\frac{1}{4\hbar}(u^2 + v^2)\right\}$	i, iii, v
Rivier	$\cos\left\{\frac{uv}{2\hbar}\right\}$	i, ii, iii, v
Standard	$\exp\left\{\frac{iuv}{2\hbar}\right\}$	i, ii, v
Weyl	1	i, ii, iii, iv, v

Table 2

In table 2 we give a comprehensive list of the well known correspondence rules along with their generating f.

4.5 ALTERNATIVES TO THE WIGNER FUNCTION

We have seen that the Wigner function is a special case of the Weyl transform, equation (1.3.15), but the Cohen function, equation (4.1.4), is not a special case of the generalised transform, equation (4.3.14). To see this we shall divide the expectation value of $\hat{\Delta}_{pqf}$ by \hbar to get, alternatively, the Cohen function for a pure state as

$$\begin{aligned} P^f(pq) &= \frac{1}{\hbar} \langle \hat{\Delta}_{pqf} \rangle \\ &= \frac{1}{\hbar} \langle \psi | \hat{\Delta}_{pqf} | \psi \rangle \end{aligned} \quad (4.5.1)$$

using equation (4.3.7) gives

$$\begin{aligned} P^f(pq) &= \frac{1}{\hbar^2} \int \exp\left\{\frac{i}{\hbar}pv\right\} \exp\left\{\frac{i}{\hbar}(q - q')\right\} f(u/\hbar, v/\hbar) \\ &\quad \times \langle q' - \frac{1}{2}v | \psi \rangle \langle \psi | q' + \frac{1}{2}v \rangle du dv dq' \\ &= \frac{1}{\hbar^2} \int \exp\left\{\frac{i}{\hbar}pv\right\} \exp\left\{\frac{i}{\hbar}(q - q')\right\} f(u/\hbar, v/\hbar) \\ &\quad \times \langle q' - \frac{1}{2}v | \hat{\rho} | q' + \frac{1}{2}v \rangle du dv dq' \end{aligned} \quad (4.5.2)$$

From equations (4.2.3) and (2.2.4) $P^f(pq)$ can be written in terms of the Wigner function as

$$P^f(pq) = f\left[\frac{1}{i}\frac{\partial}{\partial q}, \frac{1}{i}\frac{\partial}{\partial p}\right] P^W(pq) \quad (4.5.3)$$

Equation (4.5.3), at first sight, appears to be a special case of equation (4.3.19). However, for this to be true then f must automatically satisfy all the criteria of table 1. Actually, the only restraints that have been imposed upon f at this stage are $f(0,0)=1$ and the classical limit condition $f(u/\hbar, v/\hbar)=1$ when $\hbar \rightarrow 0$. This does not contradict the argument of Section 4.3 because the density matrix, $\hat{\rho}$, is an operator with unique natural properties associated with it. Thus, we can alternatively express $P^f(pq)$ by the following

$$\begin{aligned} \langle \hat{\Delta}_{pqf} \rangle &= \text{Tr} [\hat{\rho} \hat{\Delta}_{pqf}] \\ &= P^f(pq) \text{Tr} [1] \\ &= P^f(pq) \end{aligned} \quad (4.5.4)$$

where we have used equation (4.3.8).

Therefore, we are led to the conclusion that the conditions for f can be re-expressed when considering the expectation value of $\hat{\Delta}_{pqf}$. We shall now investigate this claim.

It is a reasonable requirement that the Cohen function should exhibit the same characteristics as the Wigner function. Thus, integration of equation (4.5.2) over p yields

(if $f(u/\hbar, 0)=1$)

$$\int P^f(pq) dp = |\psi(q)|^2 \quad (4.5.5a)$$

and integrating over q gives (if $f(0, v/\hbar)=1$)

$$\int P^f(pq) dq = |\varphi(p)|^2 \quad (4.5.5b)$$

hence, $P^f(pq)$ yields the correct marginals.

Following from equation (4.5.5a) or (4.5.5b) the normalisation condition is, clearly,

$$\int P^f(pq) dp dq = 1 \quad (4.5.6)$$

Since $\hat{\rho}$ is an Hermitian operator and for $P^f(pq)$ to be a real function then we must have $f^*(u/\hbar, v/\hbar) = f(-u/\hbar, -v/\hbar)$.

Since the expectation value of a quantum operator can be written as a trace then it may be required that

$$\begin{aligned} \langle \hat{A} \rangle &= \text{Tr} [\hat{A} \hat{\rho}] \\ &= \frac{1}{h} \int A^f(pq) P^f(pq) dp dq \end{aligned} \quad (4.5.7)$$

which will only be true if $f(u/\hbar, v/\hbar) f(-u/\hbar, -v/\hbar) = 1$

Thus, it is possible to motivate the same criteria on f (ie those given in table 1) by imposing reasonable conditions on $P^f(pq)$. In table 3 we list

i	$f(0,0) = 1$	Constant term of power series
ii	$f(0,v/\hbar) = f(u/\hbar,0) = 1$	Produce correct marginals
iii	$f^*(u/\hbar,v/\hbar) = f(-u/\hbar,-v/\hbar)$	$P^f(pq)$ is a real function
iv	$f(u/\hbar,v/\hbar)f(-u/\hbar,-v/\hbar) = 1$	$\text{Tr}[\hat{A}\hat{\rho}] = \frac{1}{\hbar} \int A^f(pq)P^f(pq)dpdq$
v	$\lim_{\hbar \rightarrow 0} f(u/\hbar,v/\hbar) = 1$	Classical limit

Table 3

these conditions for comparison with those in table 1. Hence, we can see how these identical conditions are arrived at by different physical arguments.

When all the conditions of f are satisfied the resulting $P^f(pq)$ assumes the characteristics of the Wigner function and becomes a special case of equation (4.3.20). We shall now only consider those f that satisfy all the criteria of table 3.

Since $P^f(pq)$ produces the correct marginals then it must as shown by Wigner, [26] assume negative values in some regions of pseudo phase space, [26]. Another way to see this is by generalising the proof of Section 2.4 property 10 as follows.

Letting ψ and φ be two orthogonal wave-functions, so that $|\langle \psi | \varphi \rangle|^2 = 0$, then we have

$$|\langle \psi | \varphi \rangle|^2 = \text{Tr} [|\psi\rangle\langle\psi| \cdot |\varphi\rangle\langle\varphi|]$$

$$= \frac{1}{h} \int P_{\psi}^f(pq) P_{\phi}^f(pq) dp dq$$

$$= 0 \quad (4.5.8)$$

Therefore, since the integral must vanish then at least one of the $P^f(pq)$ must be negative within the limits of integration.

Thus we have found that the Cohen function is subject to the same disadvantages as the Wigner function. Since the latter is obtained from the former when $f=1$ one can speculate that there is no reward in using the Cohen function as opposed to the Wigner function. In addition, the Wigner function is the simplest. To re-inforce this speculation, we now find the equation of motion of $P^f(pq)$. To do this, we need to find the generalised transform of

$$\frac{\partial \hat{\rho}}{\partial t} = \frac{\hbar}{i} [\hat{H}, \hat{\rho}] \quad (4.5.9)$$

Multiplying equation (4.5.9) on the right by $\hat{\Delta}_{pqf}$ and taking the trace gives

$$\text{Tr} \left[\frac{\partial \rho}{\partial t} \hat{\Delta}_{pqf} \right] = \frac{\hbar}{i} \text{Tr} \left[[\hat{H}, \hat{\rho}] \hat{\Delta}_{pqf} \right] \quad (4.5.10)$$

But f may also depend upon time so that the lhs of equation (4.5.10) becomes

$$\text{Tr} \left[\frac{\partial(\hat{\rho} \hat{\Delta}_{pqf})}{\partial t} - \frac{\partial f}{\partial t} \hat{\rho} \hat{\Delta}_{pqf} \right] = \frac{\partial P^f(pqt)}{\partial t} - \frac{1}{\hbar} \frac{\partial f}{\partial t} P^f(pqt) \quad (4.5.11)$$

Inserting equation (4.5.11) into (4.5.10) yields

$$\frac{\partial P^f(pqt)}{\partial t} = \frac{\hbar}{i} \{ [\hat{H}, \hat{\rho}] \}_{pq}^f + \frac{1}{\hbar} \frac{\partial f}{\partial t} P^f(pqt) \quad (4.5.12)$$

where

$$\begin{aligned} \{ [\hat{H}, \hat{\rho}] \}_{pq}^f &= \frac{2}{\hbar} H^f(pq) f \left[\frac{\overrightarrow{1\partial}}{i}, \frac{\overleftarrow{1\partial}}{i} \right]_{\partial q} f \left[\frac{\overrightarrow{1\partial}}{i}, \frac{\overleftarrow{1\partial}}{i} \right]_{\partial p} f \left[i \frac{\overleftarrow{\partial}}{\partial q} + i \frac{\overrightarrow{\partial}}{\partial q}, i \frac{\overleftarrow{\partial}}{\partial p} + i \frac{\overrightarrow{\partial}}{\partial p} \right] \\ &\times \sin \left\{ \frac{\hbar}{2} \left[\frac{\overrightarrow{\partial}}{\partial q} \frac{\overleftarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p} \frac{\overrightarrow{\partial}}{\partial q} \right] \right\} P^f(pqt) \end{aligned} \quad (4.5.13)$$

and we have used equation (4.3.25) to get equation (4.5.13).

One can now appreciate attempts to motivate the choice of the Wigner-Weyl transform from basic considerations. Clearly, in the classical limit, when $\hbar \rightarrow 0$, equation (4.5.12) reduces to the usual Liouville transport equation.

Analogous to the Wigner characteristic function, equation (2.2.7), the generalised characteristic function is given by

$$P^f(pq) = \frac{1}{\hbar^2} \int \exp \left\{ \frac{i}{\hbar} (pv + qu) \right\} C^F(u, v; f) du dv \quad (4.5.14)$$

where

$$C^F(u, v; f) = \langle \psi | f(u/\hbar, v/\hbar) \exp\left\{\frac{i}{\hbar}(\hat{p}v + \hat{q}u)\right\} | \psi \rangle \quad (4.5.15)$$

For a comparison with a discussion on another class of generalised distribution functions, [37] [38], we can set

$$f(u/\hbar, v/\hbar) = \exp\left\{\frac{s}{4\hbar}(\alpha u^2 + \beta v^2)\right\} \quad (4.5.16)$$

where α and β are constants to be determined and s takes the values 1, normal ordering, -1, anti-normal ordering, and 0, Wigner.

Inserting equation (4.5.16) into (4.5.15) gives

$$C^F(u, v; s) = \exp\left\{\frac{s}{4\hbar}(\alpha u^2 + \beta v^2)\right\} C^F(u, v) \quad (4.5.17)$$

where $C^F(u, v; s)$ is the general characteristic function generated by the allowed values of s and $C^F(u, v)$ is the Wigner characteristic function.

Substituting equation (4.5.16) into (4.5.3) gives

$$P^S(pq) = \exp\left\{-\frac{s}{4\hbar}\left[\alpha \frac{\partial^2}{\partial q^2} + \beta \frac{\partial^2}{\partial p^2}\right]\right\} P^W(pq) \quad (4.5.18)$$

The equation of motion for $P^S(pq)$ has been discussed in detail, [37] [38]. It has a complicated open structure and as been pointed out to be too cumbersome for practical applications, unless $s=0$.

However, for potentials up to and including that of the harmonic oscillator we can obtain a closed analytical form of the equation of motion of $P^s(pq)$. This is given by equations (28) and (31) of ref [38], namely

$$\begin{aligned} \frac{\partial P^s(pqt)}{\partial t} = & -\frac{1}{m} \left[p - \frac{s\beta}{4\hbar} \frac{\partial}{\partial p} \right] \frac{\partial P^s(pqt)}{\partial q} \\ & + \frac{2}{\hbar} V(q) \sin \left\{ \frac{\hbar}{2} \left[\frac{\overleftarrow{\partial}}{\partial q} \frac{\overrightarrow{\partial}}{\partial p} \right] \right\} \exp \left\{ \frac{s\alpha}{4\hbar} \left[\frac{\overleftarrow{\partial}}{\partial q} \frac{\overrightarrow{\partial}}{\partial p} \right] \right\} P^s(pqt) \end{aligned} \quad (4.5.19)$$

Taking s to be -1 in equation (4.5.16) we have, explicitly,

$$f(u/\hbar, v/\hbar) = \exp \left\{ -\frac{1}{4\hbar} (\alpha u^2 + \beta v^2) \right\} \quad (4.5.20)$$

Equation (4.5.20) generates the smoothed Wigner or Husimi function, [38]. To find this function substitute equation (4.5.20) into (4.5.1) to get

$$\begin{aligned} P^a(pq) = & \frac{1}{\hbar^2} \int \exp \left\{ \frac{i}{\hbar} p v \right\} \exp \left\{ \frac{i}{\hbar} (q - q') u \right\} \exp \left\{ -\frac{1}{4\hbar} (\alpha u^2 + \beta v^2) \right\} \\ & \times \langle q' - \frac{1}{2} v | \hat{\rho} | q' + \frac{1}{2} v \rangle du dv dq' \end{aligned}$$

evaluating the Gaussian in u gives

$$P^A(pq) = \frac{1}{h\sqrt{\alpha\pi}} \int \exp\left\{-\frac{1}{\alpha}(q - q')^2\right\} \exp\left\{-\frac{\beta v^2}{4\hbar^2} - \frac{i}{\hbar}pv\right\}$$

$$x < q' - \frac{1}{2} v | \hat{\rho} | q' + \frac{1}{2} v > dv dq'$$

$$= \frac{1}{h^2\sqrt{\alpha\pi}} \int \exp\left\{-\frac{1}{\alpha}(q - q')^2\right\} \exp\left\{-\frac{\beta v^2}{4\hbar^2} - \frac{i}{\hbar}pv\right\} \exp\left\{\frac{i}{\hbar}(v' - v)p'\right\}$$

$$x < q' \frac{1}{2} v' | \hat{\rho} | q' + \frac{1}{2} v' > dv dv' dp' dq'$$

evaluating the Gaussian in v gives

$$P^A(pq) = \frac{1}{\pi\sqrt{\alpha\beta}} \int \exp\left\{-\frac{1}{\alpha}(q - q')^2\right\} \exp\left\{-\frac{1}{\beta}(p - p')^2\right\} P^W(p'q') dp' dq' \quad (4.5.21)$$

choosing

$$\alpha = 2\sigma^2 \quad \text{and} \quad \beta = \hbar^2/2\sigma^2$$

in equation (4.5.21) gives the Husimi function

$$P^H(pq) = \int Q(p - p', q - q') P^W(p'q') dp' dq' \quad (4.5.22)$$

where

$$Q(p - p', q - q') = \frac{2}{h} \exp \left\{ -\frac{(q - q')^2}{2\sigma^2} - \frac{2\sigma^2}{h^2} (p - p')^2 \right\}$$

(4.5.23)

Thus, we have an alternative derivation to that given in [38]. Equation (4.5.22) is an example of a non-negative distribution, [35], but, of course, it does not produce the correct marginals.

BIBLIOGRAPHY

- 1 S. R. DeGroot and L. G. Suttorp, Foundations of Electrodynamics (North Holland, Amsterdam, 1972).
- 2 K. Imre, E. Ozimir, M. Rosenbaum and P. Zweifel, J. Math. Phys. 8, 1097 (1967).
- 3 a) B. Leaf, J. Math. Phys. 9, 65 (1968).
b) B. Leaf, J. Math. Phys. 9, 769 (1968).
- 4 H. J. Groenewold, Physica, 12, 405, (1946).
- 5 J. R. Shewell, Am. J. Phys. 27, 16 (1959).
- 6 L. Cohen, J. Math. Phys. 7, 781 (1966)
- 7 a) H. Weyl, Z. Phys. 46, 1 (1927).
b) H. Weyl, The Theory of Groups and Quantum Mechanics (Dover Publications, New York, 1950, p274).
- 8 A. Jannussis and N. Patargias, Phys. Lett. 53A, 357 (1975).
- 9 M. Hillary, R. F. O'Connell, M. O. Scully and E. Wigner, Physics Reports 106, No 3, 121-167 (1984).
- 10 R. M. Wilcox, J. Math. Phys. 8, 962 (1967).
- 11 L. I. Schiff, Quantum Mechanics (McGraw-Hill 3rd Edition)
- 12 A. Royer, Phys. Rev. A15, 449, (1977).
- 13 R. J. Glauber, Phys. Rev. 131, 2766, (1963).
- 14 J. G. Kruger and A. Poffyn, Physica, 85A, (1976).
- 15 H. Goldstein, Classical Mechanics (2nd Edition, Reading, Ma: Addison-Wesley, 1980).
- 16 H. Weyl, The Classical Groups, (Princeton Univ Press 1939).
- 17 M. Hall, J. Phys. A: Math. Gen. 18, 29, (1985).

- 18 E. P. Wigner, Phys. Rev. 40, 749 (1932).
- 19 J. E. Moyal, Proc. Cambr. Phil. Soc. 45, 99 (1949).
- 20 J. von Neumann, Mathematical Foundation of Quantum Mechanics (Princeton University Press, Princeton, New Jersey, 1955).
- 21 R. L. Hudson, Rept. Math. Phys. 6, 249 (1974).
- 22 F. Soto and P. Claverie, J. Math. Phys. 24, 97, (1983).
- 23 T. L. Hill, Statistical Mechanics, (McGraw-Hill Inc. 1956).
- 24 G. Baker Jnr, Phys. Rev. 109, 2198 (1958).
- 25 J. S. Kim and E. P. Wigner, Am. J. Phys. 58, 439 (1980).
- 26 E. P. Wigner, Perspectives in Quantum Theory (editors W. Youngrau and A. van der Merwe, Cambridge, Mass. and London MIT Press 25 - 36, 1971).
- 27 I. Oppenheim and J. Ross, Phys. Rev. 107, 28 (1957).
- 28 R. W. Davies and K. T. R. Davies, Ann. of Phys. 89, 261 (1975).
- 29 a) R. P. Feynmann, Rev. Mod. Phys., 20, 367 (1948).
b) R. P. Feynmann and A. R. Hibbs, Quantum Mechanics and Path Integrals (McGraw-Hill, New York, 1965).
- 30 L. S. Schulman, Techniques and Applications of Path Integration (Wiley, New York, 1981).
- 31 M. C. Wang and G. E. Uhlenbeck, Rev. Mod. Phys. 17, 323 (1945).
- 32 T. B. Smith, J. Phys. A: Math. Gen., Vol 11, No 11, (1978).
- 33 C. L. Mehta, J. Math. Phys., 5, 677, (1964).
- 34 K. Husimi, Proc. Phys. Soc. Jpn., 22, 264, (1940).
- 35 N. D. Cartwright, Physica, 83A, 210, (1976).

- 36 L. Cohen and Y. I. Zaparovanny, J. Math. Phys., 21,
794, (1980).
- 37 R. F. O'Connell and E. P. Wigner, Phys. Letts., 85A,
121, (1981).
- 38 R. F. O'connell, L. Wang and H. A. Williams, Phys. Rev.,
30, 2187, (1984).
- 39 R. F. O'connell and E. P. Wigner, Phys. Letts, 83A,
145, (1981).
- 40 T. B. Smith, Phys. Lett., 127A, 75, (1988).